Universidad Politécnica de Madrid
Escuela Técnica Superior de Ingeniería Agronómica, Alimentaria y de Biosistemas
Departamento de Ingeniería Agroforestal

**HYDROLOGICAL MODELLING AND EVAPOTRANSPIRATION
ESTIMATION BASED ON REMOTE SENSING DATA
A CASE STUDY IN THE DOÑANA REGION AND SURROUNDING
IRRIGATED AREAS**

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“Though I do not believe that a plant will spring up where no seed has been, I have great faith in a seed. Convince me that you have a seed there, and I am prepared to expect wonders”.

Henry David Thoreau, *The Dispersions of Seeds*

*A mi familia,
por educarme en el esfuerzo desde la generosidad y la humildad*

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Abstract

Water scarcity is rapidly increasing in many regions, and is expected to worsen in the coming decades. In semiarid regions, which extend over a 15% of the global land area, water is an important limitation for vegetation growth and a cause of concern for the long-term sustainability of its associated ecosystems, particularly where natural ecosystems and crops compete for the same water sources. Despite the importance of water scarcity in these regions, data availability is often limited and hydrological studies must still be improved. In order to inform water management decisions, it is crucial to assess the water balance components and particularly the evapotranspiration (*ET*), a crucial component in both the Earth water and energy balances.

In the present thesis, hydrological modelling and remote sensing (RS)-based approaches are assessed and compared to investigate the potentiality to improve the estimation of the components of the water balance, particularly the *ET*. The study is accomplished in Spain, specifically in a semiarid region subject to the application of water management actions: the World Heritage protected UNESCO Doñana region and surrounding irrigated areas, including the BXII Irrigation District (BXII ID) situated where the old Guadalquivir marshes were located.

The specific objectives were: (1) to develop a hydrological model, WATEN, aiming to assess the water balance components, (2) to deepen on the *ET* estimation through the reformulation of a RS-based *ET* model, the PT-JPL-thermal, (3) to compare the *ET* derived from WATEN, the PT-JPL-thermal model and the *ET* derived from the globally available RS-based *ET* product MOD16, and (4) to identify hot-spots of drying trends and pluri-annual periods of increasing or decreasing water use based on the spatio-temporal *ET* dynamics.

In the first study of this work, the WATEN model was developed and implemented in the BXII ID, allowing the quantification of the water balance components from 2003 to 2012, in particular *ET*, drainage and soil moisture content. The model uses an alternative calibration method based on energy consumption data at the drainage pumping stations, which is an interesting approach for areas where access to streamflow information is not available. *ET* is considered linearly reduced when the water content falls below the readily available moisture in the soil and resulting in estimates about 18% below potential values, reaching up to a 40% reduction in August.

The second study has focused on assessing *ET* patterns in the region by means of three methods: i) the locally calibrated hydrological model WATEN; ii) the RS-based PT-JPL-thermal model modified in this work and iii) the globally available RS-based *ET* product MOD16.

In the mixed-irrigation BXII, the PT-JPL-thermal showed a reasonable agreement with the WATEN *ET* estimates, both in amount and dynamics. PT-JPL-thermal estimates were a 7% higher than those from WATEN and the correlation coefficient values were $\rho = 0.78$ and $\rho_{1month-lag} = 0.9$. On the other hand, MOD16 underestimated *ET* by 40% and the correlation coefficient with WATEN was only $\rho = 0.48$. The PT-JPL-thermal and the MOD16 *ET* estimates were extended to the whole Doñana region and surrounding irrigated areas including rice fields and natural ecosystems, such as wetlands, shrublands and forests. For all the land cover classes, the PT-JPL-thermal *ET* estimations approached the documented *ET* rates in the region (both natural ecosystems and irrigated areas), whereas MOD16 underestimated *ET* in all the cases although it was able to identify *ET* spatial patterns and interannual variability.

This study has shown that the re-formulation of the outgoing longwave radiation, together with the use of the thermal inertia concept as a proxy to soil moisture content is a more appropriate approach for assessing *ET* in semiarid environments than the use of vapor pressure deficit. This variable (used by MOD16) may reflect the surrounding arid conditions but fail to consider the real values of soil water availability. In addition, the PT-JPL-thermal only requires air temperature and incoming solar radiation, apart from standard satellites-products freely available, which makes it a model that can be easily applied in areas with little availability of information.

In the third study, the PT-JPL-thermal model was used to assess the pressures on natural ecosystems and agriculture in the Doñana region, where natural ecosystems and crops compete for the same water sources, over the last 14 years, a competition that has increased as the region dries.

The *ET* was found to be correlated with precipitation in all the ecosystems, especially in the wetlands and to a lesser extent in the shrublands, forests and croplands, suggesting a more pronounced susceptibility of the wetlands to overall drying. The analysis of the *ET* trends allowed to distinguish hot-spots, that is, areas where the water used by natural ecosystems was declining or increasing throughout the study period. Moreover, our results showed the significant increase of *ET* in some areas of intensive agriculture,

which points to a greater diversion of water to the crops when the water supply has been dwindling. These results are relevant in terms of providing useful information for water management, helping in decision-making for the balance between regional demands for agriculture and environmental sustainability, and providing relevant information in the context of climatic changes.

Resumen

La escasez de agua está agravándose en muchas regiones a nivel global, y se espera que empeore en las próximas décadas. En las regiones semiáridas, que abarcan más del 15% de la superficie terrestre mundial, el agua es un factor limitante para la vegetación y para la sostenibilidad de sus ecosistemas naturales asociados, especialmente en presencia de zonas agrícolas de regadío que compiten por los mismos recursos. Por la importancia del agua en estas regiones y particularmente en áreas con datos hidrológicos limitados, los avances realizados en la estimación de magnitudes hidrológicas deben ser adaptados y perfeccionados para analizar la situación de este recurso. Para dar soporte a la toma de decisiones en materia de gestión hídrica, es crucial evaluar los componentes del balance hídrico, particularmente la evapotranspiración (*ET*), un componente fundamental en el balance hídrico y energético de la Tierra.

En la presente tesis, se proponen y evalúan modelos hidrológicos y de teledetección (RS) con objeto de mejorar la estimación de los componentes del balance hídrico. El estudio se ha llevado a cabo en España, en particular en una región semiárida sujeta a la posible aplicación de medidas en materia de gestión hídrica: la región Patrimonio Mundial de la UNESCO de Doñana, y las zonas de regadío circundantes, incluido el Sector BXII localizado donde se encontraban las antiguas marismas del Guadalquivir. Para ello, se establecieron los siguientes objetivos específicos: (1) desarrollar un modelo hidrológico, WATEN, con el objetivo de evaluar los componentes del balance hídrico, (2) profundizar en la componente de evapotranspiración a través de la reformulación de un modelo basado en teledetección, el modelo PT-JPL-thermal, (3) comparar la *ET* derivada del modelo hidrológico WATEN, la *ET* derivada del modelo PT-JPL-thermal y la *ET* derivada del producto global de NASA para la *ET*, MOD16 y (4) analizar la dinámica espacio-temporal de la evapotranspiración en el área de estudio basada en los modelos propuestos, identificando zonas concretas de tendencias secas junto con períodos plurianuales de uso creciente o decreciente del agua.

En el primer estudio, se desarrolló un modelo hidrológico conceptual, WATEN, que se aplicó al sector de riego BXII y permitió estimar las series mensuales de drenaje, evapotranspiración y contenido de humedad del suelo durante el periodo de estudio 2003-2012. WATEN propone una calibración alternativa basada en los consumos

energéticos de las estaciones de bombeo de drenaje. Este enfoque resulta de interés en áreas donde no existe información sobre caudales y en las que, sin embargo, de haber bombeos, sus consumos energéticos quedan registrados. WATEN considera que la *ET* se reduce linealmente cuando el contenido de agua disminuye por debajo del umbral fácilmente disponible, y resultó en estimaciones de un 18% por debajo de los valores potenciales, alcanzando hasta un 40% de reducción en el mes de agosto.

El segundo estudio se ha centrado en la evaluación de los patrones de *ET* en la región: i) el modelo hidrológico calibrado *in situ* WATEN; ii) el modelo PT-JPL-thermal basado en RS y modificado en este trabajo y iii) el producto de *ET* basado en RS, MOD16, disponible globalmente.

En el Sector BXII, el modelo PT-JPL-thermal mostró concordancia con las estimaciones de *ET* derivadas de WATEN, tanto en términos cuantitativos como en sus dinámicas. Las estimaciones del PT-JPL-thermal resultaron un 7% mayores que las de WATEN y los coeficientes de correlación fueron $\rho = 0.78$ y $\rho_{1\text{month-lag}} = 0.94$. MOD16 subestimó la *ET* en un 40% y el coeficiente de correlación frente a WATEN fue $\rho = 0.48$. Las estimaciones de PT-JPL-thermal y MOD16 *ET* se extendieron a toda la región de Doñana y las áreas de regadío circundantes, incluidos los arrozales, y los ecosistemas naturales de humedales, matorrales y bosque. Para todas las clases de cobertura de suelo, las estimaciones de *ET* del PT-JPL-thermal se ajustaron a las dinámicas de *ET* documentadas en la región (ecosistemas naturales y zonas regadas), mientras que MOD16 subestimó la *ET* en todos los casos, aunque pudo identificar patrones espaciales *ET* y variabilidad interanual.

Este estudio ha demostrado que la reformulación de la radiación neta, junto con el uso del concepto de inercia térmica como indicador del contenido de humedad del suelo, es un enfoque más apropiado para evaluar *ET* en ambientes semiáridos que el uso del déficit de presión de vapor. Esta variable (utilizada por MOD16) puede reflejar las condiciones áridas circundantes, pero no considera los valores reales de la disponibilidad de agua en el suelo. Además, el PT-JPL-thermal requiere únicamente la temperatura del aire y la radiación solar entrante, aparte de producto satelitales estándar de libre acceso, lo que le convierte en un modelo que se puede aplicar fácilmente en áreas con reducida disponibilidad de información.

En el tercer estudio, el modelo PT-JPL-thermal fue eficaz para ayudar a comprender las presiones sobre los ecosistemas naturales y la agricultura que la región de Doñana,

donde los ecosistemas naturales y los cultivos compiten por las mismas fuentes de agua, ha experimentado en los últimos 14 años, una competencia que ha aumentado a medida que los recursos hídricos escasean.

La *ET* resultó altamente correlacionada con la precipitación en las zonas de marisma, y en mucha menor medida en los matorrales, bosques y tierras de cultivo, lo que sugiere una susceptibilidad más pronunciada de los humedales a la escasez hídrica, aunque toda la región es susceptible. El análisis de las tendencias de *ET* permitió distinguir las áreas donde el uso del agua para los ecosistemas naturales ha disminuido y las zonas donde el uso del agua ha aumentado significativamente a lo largo del período de estudio. Por otro lado, la investigación encontró que la *ET* aumentó en algunas zonas de agricultura intensiva, lo que apunta a una mayor desviación de agua hacia los cultivos cuando la escasez de agua ha sido más acuciada. Estos resultados son relevantes en cuanto que aportan información útil para la gestión hídrica, ayudando en la toma de decisiones hacia un equilibrio entre las demandas regionales agrícolas y la sostenibilidad ambiental, y proporcionando información relevante en el contexto del cambio climático.

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List of symbols

$ASMD$	Auxiliary SMD variable to facilitate WATEN calculations [mm]
ATI	Apparent thermal inertia [K^{-1}]
$biolim$	Biophysical limitation [-]
C	Coefficient to consider the solar flux variation as a function of latitude [-]
c	Constant in the instantaneous longwave radiation formulation [0.261] Time lag coefficient for the minimum air temperature after sunrise [h]
C_{ET}	Crop evapotranspiration coefficient [-]
c_p	Specific heat at constant pressure [$MJ\ kg^{-1}\ ^\circ C^{-1}$]
C_L	Mean stomatal conductance per unit LAI [$m\ s^{-1}$]
C_S	Stomatal conductance [$m\ s^{-1}$]
$CUDM$	Unitary cumulative deviations from the mean [-]
CV	Coefficient of variation [-]
d	Zero plane displacement of wind profile due to the presence of canopy [m] Constant in the instantaneous longwave radiation formulation [7.77×10^{-4}] Time lag coefficient for the maximum air temperature before sunset [h]
D	Drainage [mm]
e	Actual vapor pressure [kPa]
e^o	Saturation vapor pressure at air temperature T [kPa]
E	Energy consumption [$W\ h\ m^{-3}$]
E_D	Energy consumption derived from drainage in WATEN [$W\ h\ m^{-3}$]
E_u	Energy consumption per unit volume [$kW\ h\ m^{-3}$]
$Emis$	Emissivity [-]
ET	Evapotranspiration [mm]
ET_c	Potential crop evapotranspiration [mm]
ET_o	Reference evapotranspiration [mm]
ET_p	Potential evapotranspiration [mm]
EVI	Enhanced vegetation index [-]
f	Soil evaporation factor [-]
f_{APAR}	Absorbed photosynthetically active radiation fraction [-]
f_{IPAR}	Intercepted photosynthetically active radiation fraction [-]

f_g	Green canopy fraction [-]
f_m	Plant moisture constraint [-]
f_{sm}	Soil moisture constraint [-]
f_t	Plant temperature constraint [-]
f_o	Initial crop development stage [day]
f_4	Final crop development stage [day]
G	Soil heat flux [$\text{MJ m}^{-2} \text{ day}^{-1}$]
G_c	Canopy conductance [m s^{-1}]
G_s	Surface conductance ($1/r_s$) [m s^{-1}]
G_{smin}	Surface conductance controlling soil evaporation [m s^{-1}]
g_{sx}	Maximum stomatal conductance [m s^{-1}]
H	Sensible heat flux [$\text{MJ m}^{-2} \text{ day}^{-1}$]
I	Irrigation [mm]
J	Auxiliary variable to transform instantaneous into daily radiation [-]
k	Von Karman's constant [0.41] [-]
K_c	Crop coefficient [-]
K_{cb}	Basal crop coefficient [-]
k_{rn}	Constant in the soil net radiation formulation [0.6]
L_{ini}	Length of initial growth stage [day]
L_{dev}	Length of crop development growth stage [day]
L_{mid}	Length of mid-season growth stage [day]
L_{end}	Length of late season growth stage [day]
LAI	Leaf area index [-]
LST	Land surface temperature [K]
m	Mass for moist air [kg m^{-3}] Time elapsed from minimum daily temperature until sunset [h]
m_v	Mass for vapor [kg m^{-3}]
MAE	Mean absolute error [-]
VPD	Vapor pressure deficit [kPa]
$MODIS_{time}$	Time for MODIS overpass [h]
N	Elapsed time between sunrise and sunset from NOAA [h]
n_p	Number of pairs [-]
$NDVI$	Normalized difference vegetation index [-]

p	Atmospheric pressure [kPa]
	Evapotranspiration depletion factor [-]
	p value [-]
P	Precipitation [mm]
PAR	Photosynthetically active radiation [W m^{-2}]
q_h	Specific humidity [-]
Q_L	Latent heat [J]
Q_S	Sensible heat [J]
r_a	Aerodynamic resistance [s m^{-1}]
r_s	Surface or canopy resistance [s m^{-1}]
R_a	Specific universal constant for dry air [$\text{kJ kg}^{-1} \text{K}^{-1}$]
R_I	Fraction of effective irrigation [-]
R_L	Longwave radiation [W m^{-2}]
$R_L^\downarrow$	Incoming longwave radiation [W m^{-2}]
$R_{Linst}^\downarrow$	Instantaneous incoming longwave radiation [W m^{-2}]
$R_L^\uparrow$	Outgoing longwave radiation [W m^{-2}]
R_n	Surface net radiation [$\text{MJ m}^{-2} \text{day}^{-1}$]
R_{nc}	Daily canopy net radiation [W m^{-2}]
R_{ns}	Daily soil net radiation [W m^{-2}]
Rl_a	Longwave radiation absorbed by the surface from the atmosphere [$\text{MJ m}^{-2} \text{day}^{-1}$]
Rl_e	Longwave radiation emitted from the surface to the atmosphere [$\text{MJ m}^{-2} \text{day}^{-1}$]
Rl_n	Net longwave radiation absorbed by the surface [$\text{MJ m}^{-2} \text{day}^{-1}$]
Rl_{out}	Outgoing longwave radiation emitted by the surface and the atmosphere [$\text{MJ m}^{-2} \text{day}^{-1}$]
R_p	Fraction of effective precipitation [-]
R_s	Shortwave radiation that reaches the surface [$\text{MJ m}^{-2} \text{day}^{-1}$]
$R_S^\downarrow$	Incoming shortwave radiation [W m^{-2}]
$R_S^\uparrow$	Outgoing shortwave radiation [W m^{-2}]
R_{Sday}	Daily shortwave radiation [W m^{-2}]
$R_{Sday}^\downarrow$	Daily incoming shortwave radiation [W m^{-2}]
RS_{in}	Incoming shortwave radiation [$\text{MJ m}^{-2} \text{day}^{-1}$]

R_{Sinst}	Instantaneous shortwave radiation [W m^{-2}]
Rs_n	Net shortwave radiation absorbed by the surface [$\text{MJ m}^{-2} \text{ day}^{-1}$]
Rs_{out}	Outgoing shortwave radiation reflected [$\text{MJ m}^{-2} \text{ day}^{-1}$]
RAM	Readily available moisture [mm]
$Ref0$	Parametric vector initially considered in WATEN [-]
RH	Relative humidity [%]
$RMSE$	Root mean square error [-]
S	Soil moisture content [mm]
S_M	Maximum soil moisture content [mm]
SMC	Soil moisture content [mm]
SMD	Soil moisture deficit [mm]
$STDA$	Standardized anomalies [-]
T	Temperature [$^{\circ}\text{C}$]
T_a	Air temperature [$^{\circ}\text{C}$]
$T_{air_{MODIS_{time}}}$	Air temperature at the time of MODIS overpass [$^{\circ}\text{C}$]
T_{aero}	Temperature which when combined with T_a and a resistance from the log-profile, provides an estimate of the surface sensible heat flux [$^{\circ}\text{C}$]
T_{am}	Mean air temperature [$^{\circ}\text{C}$]
T_{opt}	Optimum air temperature for plant development [$^{\circ}\text{C}$]
T_S	Land surface temperature acquired from MYD11A2 [K]
TAM	Total available moisture [mm]
TI	Thermal inertia [$\text{W m}^{-2} \text{ K}^{-1} \text{ s}^{1/2}$]
u_z	Wind speed at z m above ground surface [m s^{-1}]
V	Vertical wind speed [m s^{-1}]
$\bar{V}$	Mean vertical wind speed [m s^{-1}]
V_I	Total monthly irrigation [m^3]
VI	Vegetation index [-]
WDI	Water deficit index [-]
z_h	Height of air humidity measurements [m]
z_{oh}	Roughness length, heat and water vapor (height at which the flow is zero in the heat and water vapor logarithmic profile) [m]
z_{om}	Roughness length, momentum (height at which the speed is zero in the wind logarithmic profile) [m]

z_v	Height of wind speed measurements [m]
λ	Latent heat of vaporization [MJ kg ⁻¹]
λE	Latent heat flux [MJ m ⁻² day ⁻¹] or [W m ⁻²]
λE_c	Latent heat flux of the canopy transpiration [W m ⁻²]
λE_p	Potential latent heat flux [W m ⁻²]
$\lambda E p_c$	Potential canopy transpiration heat flux [W m ⁻²]
$\lambda E p_s$	Potential soil evaporation heat flux [W m ⁻²]
λE_s	Soil evaporation heat flux [W m ⁻²]
$\lambda E T_c$	Potential crop evapotranspiration heat flux [W m ⁻²]
$\lambda E T_o$	Reference evapotranspiration heat flux [W m ⁻²]
α	Shortwave reflectance coefficient or albedo [-]
a_{BSA}	Broadband black-sky albedo [-]
a_{WSA}	Broadband white-sky albedo [-]
α_{PT}	Priestley-Taylor empirical multiplier [-]
γ	Psychrometric constant [kPa °C ⁻¹]
Δ	Slope of saturation vapor pressure-temperature curve [kPa °C ⁻¹]
β	Bowen ratio [-]
ρ	Air density [kg m ⁻³]
σ	Correlation coefficient [-]
	Stefan-Boltzmann constant [5.67×10 ⁻⁸ W m ⁻² K ⁻⁴]
	Standard deviation [-]
ε_s	Average emissivity from MODIS bands 31 and 32 [-]
ϑ	Latitude [radians] [-]
φ	Solar declination [radians] [-]
Δz	Geometric height [m]
Δz_p	Project geometric height [m]
e_2	Nash-Sutcliffe coefficient of efficiency [-]
U	Theil's inequality coefficient [-]
u_m	Theil's variance [-]
u_s	Theil's covariance [-]
u_c	Theil's proportions [-]

Subscripts

<i>a</i>	Air
<i>c</i>	Canopy
<i>max</i>	Maximum values
<i>mean</i>	Mean values
<i>min</i>	Minimum values
<i>s</i>	Soil

List of abbreviations

BXII-ID	BXII Irrigation District
CHG	Confederación Hidrográfica del Guadalquivir
CRR	Conceptual Rainfall-Runoff
EC	Eddy Covariance
EO	Earth Observation
EOSDIS	Earth Observing System Data and Information System
EU	European Union
FAO	Food and Agriculture Organization of the United Nations
HM	Hydrological Model
LSM	Land Surface Model
FAO	Food and Agricultural Organization of the United Nations
IFAPA	Instituto de Investigación y Formación Agraria y Pesquera
INC	Instituto Nacional de Colonización
IPCC	Intergovernmental Panel on Climate Change
IRYDA	Instituto Nacional de Reforma y Desarrollo Agrario
JdA	Junta de Andalucía
MCS	Monte Carlo Simulation
MODIS	Moderate Resolution Imaging Spectroradiometer
MOD16	MODIS Global Terrestrial Evapotranspiration (<i>ET</i>) Product
NASA	National Aeronautics and Space Administration
NOAA	National Oceanic and Atmospheric Administration
PAR	Photosynthetically Active Radiation
PEDT	Parameters Estimation based on Driven Trials
PM	Penman-Monteith
PT	Priestley and Taylor
PT-JPL	Priestley-Taylor Jet Propulsion Laboratory Model
PT-JPL-thermal	Thermal version of the PT-JPL Model
RIAA	Red de Información Agroclimática de Andalucía
RS	Remote Sensing
SEB	Surface Energy Balance
SIOSE	Sistema de Información sobre Ocupación del Suelo de España
UNESCO	United Nations Educational, Scientific and Cultural Organization

VBA	Visual Basic for Applications
WFD	Water Framework Directive
WWAP	World Water Assessment Programme
WWF	World Wildlife Fund

CHAPTER 1

Introduction

1 Introduction

1.1 Research context

This dissertation has been accomplished to fulfill the requirements of the Agro-Engineering doctorate programme at the *Universidad Politécnica de Madrid (UPM)*, and has been partially funded by a Spanish FPI research fellowship programme granted by the *Centro de Estudios Hidrográficos (CEH)*, CEDEX ([BOE núm. 291 de 2010](#)). In addition, this research has been granted by the FORWARD project and the COST action EURO-AGRIWAT (<http://www.cost.eu>) with a research stay in the Department of Environmental Engineering at Denmark Technical University (DTU). The dissertation has been supervised by the professors Dr. Luis Juana Sirgado (Hydraulics, Hydrology and Irrigation Unit, Department of Agroforestry Engineering) and Dr. Alicia Palacios Orueta (Department of Systems and Natural Resources). This PhD dissertation has been developed in collaboration with the professors Dr. Mónica García from DTU and Dr. Joshua Fisher from the NASA Jet Propulsion Laboratory, California Institute of Technology.

1.2 Problem description

Anthropogenic pressure on land and water resources is stretching the planet's sustainability to its limits (Rockström *et al.*, 2009) due to the lack of land and water resources to cope with food security in an increasing world population (Bastiaanssen and Steduto, 2017). Water scarcity is rapidly increasing in many regions, and is expected to worsen in the coming decades (Vörösmarty *et al.*, 2000). Currently, about 900 million people live in water-scarce river basins, while other 700 million live in areas approaching water-scarce scenarios (Molden D. *et al.*, 2007).

The overexploitation of freshwater resources threatens food security (Kummu *et al.*, 2016) in a world where agriculture accounts for about 60 to 90% of water withdrawals mostly through irrigation (Bastiaanssen and Steduto, 2017), and where agricultural outputs are expected to increase by 50% to feed a population of 9 billion by 2050 (Muller *et al.*, 2017). Thus it is becoming increasingly important to ensure the sustainability of freshwater resources through the use of management strategies that usually require hydrological monitoring and modelling of the terrestrial water budget (Herman *et al.*, 2018).

In semiarid regions, which extend over 15% of the global land area, water is the main constraint for vegetation growth and a cause of concern for the long-term sustainability of its associated ecosystems (Fensholt *et al.*, 2012). In these regions, since irrigated agriculture uses about 80% of fresh water (Dehghanisanij *et al.*, 2006), an accurate assessment of the available and renewable water resources is one of the more urgent challenges (UNESCO, 2016). However, despite the importance of water scarcity in these areas and the significant number of studies, the quantification of the hydrological cycle must still be improved. Often these areas are classified as ungauged basins due to limited hydrological data (Andersen, 2008).

Out of the total precipitation worldwide, only one third reaches the oceans (Sumner and Jacobs, 2005) while two-thirds infiltrate into the soil (green water) and return to the atmosphere as evapotranspiration (*ET*). This component has a strong effect in the magnitude and variability of the catchment water yield (Zhang *et al.*, 2008; Zhang *et al.*, 2010) and plays a crucial role in the Earth water and energy balances at global level.

Understanding the different factors involved in the *ET* dynamics and the identification of hot-spots of drying trends is key for the formulation of water management policies, particularly in arid and semiarid regions where intensified agricultural management, land use modifications and climatic changes have derived on noticeable shifts on the terrestrial eco-hydrological processes. In this context, the study of the water fluxes trends, particularly *ET*, is essential in the diagnosis of the water cycle intensification (Mo *et al.*, 2017).

Point-scale *ET* estimations have been traditionally carried out as a residual of the water balance or, when available, through meteorological equipment measurements. When streamflow data is available, it serves to close the water balance and to calibrate hydrological *ET* models, although meteorological and streamflow information are not always available and it is frequent to find no or missing data (Turner, 1989).

Traditionally, when no other information is available, estimates of reference or potential *ET* values (i.e. Penman-Monteith and Priestley-Taylor) are reduced to actual *ET* by considering the soil moisture content (*SMC*) (Kite and Droogers, 2000). This variable is maybe the main constraint in the evapotranspiration process and its monitoring is a common practice at small-spatial scale hydrological modelling (Herman *et al.*, 2018). At larger scales the feasibility to track *SMC* is reduced and in addition the large amount of data increases the complexity of the calibration process. Big data approaches relying

on RS data availability that allow a precise characterization of *SMC* at medium or large-scale studies are decisive for an adequate monitoring and management of the water resources at variable spatio-temporal scales.

Hydrological models, from lumped conceptual catchment models to more complex distributed and physically-based models, are excellent tools to characterize the water balance components, amongst them *ET*, at large scales. With the increasing complexity of hydrological modelling approaches, new data-sets that facilitate spatially explicit estimations are essential (Parajuli *et al.*, 2018) particularly in semiarid regions where these studies represent a growing field of research.

The information provided by remote sensing has increased in the last decades, including data sets needed to obtain spatial estimations of hydrological parameters, such as soil moisture, without the need of field measurements (Parajuli *et al.*, 2018).

Satellite multi-spectral information makes it possible to estimate *ET* based on surface-energy balance (SEB) equations, decreasing the need of field measurements such as *SMC*, not easily available (Bastiaanssen and Steduto, 2017). Actual *ET* is therefore estimated using SEB equations with remote sensing-based data (e.g. land surface temperature *LST*) as proxies of *SMC*. These models need less a priori information on soil and vegetation features, as well as a smaller number of ground measurements, allowing for the estimation of water fluxes over regions with lack of availability of data (Yilmaz *et al.*, 2014).

1.3 Objectives of the research

Accurate evapotranspiration estimates have a direct effect on the reduction of the terrestrial water balance uncertainties, crucial for modelling the land-water surface and its interaction with the atmosphere, and vital for sustainable water management strategies and planning, particularly in arid and semiarid areas.

The main objective of this work is to investigate the potentiality to improve the estimation of the components of the water balance, particularly the evapotranspiration *ET*, in an area subject to the possible application of water management actions. First, an original hydrological model that considers the *ET* as a function of the soil moisture content *SMC* is developed, and second, *ET* models incorporating satellite time series images are adjusted and implemented.

Although the methodology of this study pursues a general validity, its application to a real case is consubstantial to demonstrate its applicability. In particular, we selected the World Heritage protected UNESCO Doñana region and surrounding irrigated areas, including the BXII Irrigation District (BXII ID) situated where the old Guadalquivir marshes were located.

To accomplish the main goal of the study, the following specific objectives are established:

- To formulate an original hydrological model and calibrate its parameters in the BXII Irrigation District of the ancient Guadalquivir marshes. This District has specific conditions for the development of an original hydrological model that considers the evolution of the *SMC* in the soil.
- To implement a RS-based *ET* model based on the Priestley-Taylor equation with a reformulation of model net radiation in the BXII ID, extending the study to the whole Doñana region and the adjoining irrigated areas.
- To compare the *ET* results derived from the hydrological model, the proposed RS-based model and the RS-based *ET* product MOD16 based on Penman-Monteith offered by NASA.
- To analyze the spatio-temporal *ET* dynamics in the study area based on the proposed models, identifying hot-spots of drying trends and pluri-annual periods of increasing or decreasing water use.

1.4 Structure of the thesis

This thesis is structured as follows:

- Chapter 2 presents an overview of hydrological modelling, and deepens on the evapotranspiration as a component of both the hydrological and surface energy balances. This chapter introduces the physical principles of evapotranspiration and discusses the advances and the state of the art on *ET* estimations based on physical and empirical remote-sensing approaches.
- Chapter 3 describes the study areas where this study has been developed and summarizes the main methodologies implemented in the development of the thesis.
- Chapter 4 introduces the main results of this thesis, presented in three specific studies with their corresponding discussion:

- 4.1. Study I. Water balance and flow rate discharge on a receiving water body: application to the BXII Irrigation District in Spain.
 - 4.2. Study II. Vegetation water use based on a thermal and optical remote sensing model in the Mediterranean region of Doñana.
 - 4.3. Study III. Increasing competition for water between crops and wetlands as the land dries: a case study in the Doñana region, Spain.
- Chapter 5 summarizes the main conclusions of the methods and results of this thesis and the paths for future research.

A conceptual scheme is included in Fig. 1.1 to facilitate the understanding of the thesis structure:

Figure 1.1 Scheme of the thesis structure.

1.5 Publications

The core results of this thesis are either published or under revision in scientific journals and national and international congresses.

Study I

- **Moyano, M. C.**, Tornos, L., & Juana, L. (2015). Water balance and flow rate discharge on a receiving water body: Application to the BXII Irrigation District in Spain. *Journal of Hydrology*, 527, 38-49.

<https://doi.org/10.1016/j.jhydrol.2015.04.027>

- **Moyano, M. C.**, Tornos, L., & Juana, L. (2014, June). Cálculo del volumen evacuado a una masa de agua. Aplicación al Sector BXII de la Zona Regable del Bajo Guadalquivir. XXXII Congreso Nacional de Regadíos.
- **Moyano, M. C.**, Tornos, L., & Juana, L. (2014, May). A model for water discharge based on energy consumption data (WATEN). In EGU General Assembly Conference Abstracts (Vol. 16, p. 783).

<http://adsabs.harvard.edu/abs/2014EGUGA..16..783M>

Study II

- **Moyano, M.C.**, García, M., Palacios-Orueta, A., Tornos, L., Fisher, J.B., Fernandez, N., Recuero, L. & Juana, L. (2018, under review in Remote Sensing Special Issue on “Advances in the Remote Sensing of Terrestrial Evaporation” http://www.mdpi.com/journal/remotesensing/special_issues/evaporation_rs).

Vegetation water use based on a thermal and optical remote sensing model in the Mediterranean region of Doñana.

- **Moyano, M. C.**, García, M., Tornos, L., Recuero, L., Palacios-Orueta, A. & Juana, L. (2015). Assessing regional crop water demand using a satellite-based combination equation with a land surface temperature component. In EGU General Assembly Conference Abstracts (Vol. 17, p. 15503).

<http://adsabs.harvard.edu/abs/2015EGUGA..1715503M>

Study III

- **Moyano, M.C.**, García, M., Juana, L., Tornos, L., Fisher, J.B., Fernandez, N., Recuero, L. & Palacios-Orueta, A. (2018, under internal co-authors' revision). Increasing competition for water between crops and wetlands as the land dries: a case study in the Doñana region, Spain.

This thesis has been developed within the context of a Spanish FPI research fellowship in the field of sustainable water management. Ancillary results in environmental resources management have been published in close-collaboration:

- Tornos, L., Domínguez, J. A., **Moyano, M. C.**, Recuero, L., Cicuéndez, V. & Palacios-Orueta, A. (2018). Assessment of spectral indices time series for mapping rice ecosystems in the Mediterranean Region (under review in Journal of Photogrammetry and Remote Sensing).
- Recuero, L., Litago, J., Huesca, M., Pinzon, J.E., Cicuéndez, V., **Moyano, M.C.** & Palacios-Orueta, A. (2018, June). Global vegetation seasonal patterns assessment based on statistical NDVI time series analysis. IEEE YP Conference on Remote Sensing.
- Tornos, L., Huesca, M., Domínguez, J.A., **Moyano, M.C.**, Cicuéndez, V., Recuero, L. & Palacios-Orueta, A (2015). Assessment of MODIS spectral indices for determining rice paddies agricultural practices and hydroperiod. Journal of Photogrammetry and Remote Sensing 101,110-124.
<https://doi.org/10.1016/j.isprsjprs.2014.12.006>
- Tornos, L., **Moyano, M. C.**, Huesca, M., Cicuendez, V., Recuero, L., Domínguez, J. A., & Palacios-Orueta, A. (2014, May). Analysis and assessment of Shortwave Angle and Slope Index for monitoring rice phenology and hydroperiod. In EGU General Assembly Conference Abstracts (Vol. 16, p. 14304).
<http://adsabs.harvard.edu/abs/2014EGUGA..1614304T>

CHAPTER 2

Background

2 Background

2.1 An overview of hydrological modelling

The term hydrology deals with the relationship of water with the environment in each phase of the hydrologic cycle. The continuous movement of water from evaporation processes to condensation, precipitation and flows, describes the water cycle on Earth, a closed-loop system where only one third of precipitation becomes runoff and recharges the aquifers, the so called blue water that ends-up in the ocean (Hoff *et al.*, 2010).

Figure 2.1 Earth's hydrological cycle.

The continuous improvement of the available information tools and the increasingly deep knowledge of the physical environment have allowed addressing hydrological problems to a greater extent (Ruiz-García, 1999). Hydrological models represent a simplified approximation to the hydrological system, relying on mathematical equations to solve water resources at different scale-units (Seiller *et al.*, 2017). Hydrological models present different uncertainties in the inputs needed, in the conceptual modelling of the underlying processes and in model parameters (non-uniqueness solution). Generally, hydrological models are classified into: i) empirical models (black-box models or input-output models) which rely on a series of equations and average data of the catchment, ii) theoretical models (white-box models or physically-based models) based on physical laws that require powerful computer tools for its resolution and iii) conceptual models (grey-box models), intermediate between the theoretical and empirical models. These account for a simplified representation of the physical processes and simulate the hydrological behavior by establishing equations of water balance and mass transfer (Ruiz-García, 1999).

With more or less success, hydrological models allow to simulate the process of runoff generation from climate data and play an important role in hydrological planning processes. As taken from Xu (2002), the first rainfall-runoff models in the 1920s were based on a simple technique to estimate the discharge from small catchments. A large number of conceptual rainfall-runoff models followed in the 1960s to achieve a physical interpretation of the catchment behaviour, where each component of the hydrological cycle was represented by interconnected conceptual elements, e.g. the Sacramento Model (Burnash *et al.*, 1973). To forecast the effects of spatially variable inputs and outputs or the effects of land use changes among others, physically-based models with distributed parameters emerged in the 1980s. Major advances in modelling by linking them with digital elevation models and other satellite-based data e.g. vegetation cover or soil moisture patterns, have opened up the path for major advances in hydrological modelling. The different approaches differ in (i) the type and spatial extent of the application; (ii) the remote sensing data used and (iii) the micro-meteorological or land cover data needed.

2.2 Evapotranspiration as a component of the hydrological balance

The evapotranspiration ET is one of the most important components of the hydrological cycle and is an essential component in the study of hydrological processes. It combines two different and simultaneous processes, the transfer of water vapor into the atmosphere by vegetation transpiration and by soil evaporation. When the crops develop, water is predominantly lost by soil evaporation, but when the crops are well developed, transpiration becomes the main process (Allen *et al.*, 1998). Transpiration is the loss of water by plants to the atmosphere, mainly through stomata. It depends on the type of crop and its stage of development. On the surface of the ground, the soil loses water by evaporation through the pores of the surface that hold moisture content. Evapotranspiration varies according to climate and crop, usually expressed in units of water depth (i.e. the volume of evaporated water per area per time mm/day). Water depth can be also expressed in terms of energy, referring to the energy or heat that is needed to vaporize water, namely the latent heat of vaporization (λ). λ depends on temperature (i.e. at $T=20^{\circ}\text{C}$, $\lambda = 2.45$ MJ to vaporize 1kg or 0.001 m^3 , which is equivalent to 2.45 MJ m^{-2} to vaporize 1mm of water), and which can be also expressed as λE ($\text{MJ m}^{-2}\text{ day}^{-2}$).

2.3 Evapotranspiration as a component of the surface energy balance

The energy emitted from the Sun as shortwave radiation is either reflected to space or is absorbed by the atmosphere and the surface of the Earth. The heat generated is released as longwave radiation (thermal radiation), some of which radiates back into space from the upper atmosphere. Most of the emitted longwave radiation warms the lower atmosphere and thereafter, the surface of the Earth, from which radiation is mostly absorbed by greenhouse gases in the lower atmosphere. In turn, the lower atmosphere emits longwave radiation towards the surface, keeping a stable temperature and climate in the Earth.

Figure 2.2 Scheme of the Earth's energy balance.

Where:

- Rs_{in} Incoming shortwave radiation
- Rs Shortwave radiation that reaches the surface
- $\alpha \cdot Rs$ Shortwave radiation reflected; α albedo (vegetation: 0.20-0.25; bare soil: 0.05)
- Rs_n Net shortwave radiation absorbed by the surface, $Rs - \alpha \cdot Rs$
- Rs_{out} Outgoing shortwave radiation reflected by the surface and the atmosphere
- RL_a Longwave radiation absorbed by the surface from the atmosphere
- RL_e Longwave radiation emitted from the surface to the atmosphere
- RL_n Net longwave radiation absorbed by the surface $RL_a - RL_e$
- RL_{out} Outgoing longwave radiation emitted by the surface and the atmosphere

At the Earth surface, net radiation R_n is the available energy that results from the sum of shortwave and longwave radiation. R_n is transferred to the atmosphere by i) warming the evaporating surface G , soil heat flux, ii) warming the air in contact with the evaporating surface H , sensible heat flux, iii) converting liquid water to vapor λE , latent heat flux (Kalma *et al.*, 2008). The surface energy balance is based on solving the surface energy equation (Eq. 2.1).

$$R_n - G = \lambda E + H \quad (2.1)$$

Figure 2.3 Scheme of the surface energy balance.

Where:

- R_n Surface net radiation
- G Soil heat flux, positive if the soil is warming
- H Sensible heat flux, positive if the air is warming
- λE Latent heat flux, positive during evaporation.

2.4 Physical principles of evapotranspiration

A mass of air can be defined by the water vapor pressure e and temperature T . The total heat content of the air is the sum of sensible heat H , dependent on temperature, and latent heat λE , which depends of vapor pressure. In thermodynamics, the amount of energy that a mass of humid air needs to pass from condition A (T_A-e_A) to condition D (T_D-e_D) is independent from the path chosen. Fig. 2.4 illustrates the fictitious evolution path A-B-C-D (where A to B and C to D occur under adiabatic conditions) which shows the exchanges of heat produced in the process (Juana, 2001-2018).

Figure 2.4 Change in the water vapor properties in the study of evaporation.

Starting from A (e_A, T_A), the air gets saturated by cooling from point A to B (slope $-\gamma$), decreasing its sensible heat (Q_S) -lower temperature- while increasing its latent heat (Q_L) -higher vapor pressure- in the same quantity, $dQ_{A-B} = 0$.

Considering the specific humidity q_h as the mass of water vapor m_v per unit mass of moist air m :

$$q_h = \frac{m_v}{m} = 0.622 \cdot \frac{e}{p}; \quad m_v = \frac{m \cdot 0.622 \cdot e}{p} \quad (2.2)$$

Where e is the vapor pressure in kPa, p is the total atmospheric pressure in kPa and 0.622 is the ratio of the molecular mass of water to the apparent molecular mass of dry air.

When a mass of humid air moves from point A to point B, it results:

$$dQ_L = \lambda \cdot dm_v = \frac{\lambda \cdot m \cdot 0.622}{p} \cdot de = -dQ_S = -m \cdot c_p \cdot dT; \quad (2.3)$$

Where λ is the latent heat of evaporation, i.e. the energy required to change the state of water from liquid to vapor, dependent on temperature. An empirican expression to estimate λ is:

$$\lambda_{kJ/kg} = 2491 - 2.13 \cdot T(^{\circ}C) \quad (2.4)$$

$$\text{Where } de = \frac{p \cdot c_p}{\lambda \cdot 0.622} \cdot dT = -\gamma \cdot dT$$

Where $c_p = \frac{\lambda \cdot 0.622 \cdot \gamma}{p} = 0.2396 \text{ cal/g}^\circ\text{C} = 1013 \text{ J/kg}^\circ\text{C}$, specific heat at constant pressure.

Where γ is the psychrometric constant, the slope of the path followed from A to B.

Resulting $e_B^o - e_A = \gamma \cdot (T_A - T_B)$ when the air changes from point A to B conditions.

Each unit of volumetric air that changes from point A to point B conditions, loses sensible heat $[\rho \cdot c_p \cdot (T_A - T_B)] \text{ (kJ/m}^3\text{)}$ and gains latent heat. To study the diffusion of water vapor from an evaporating surface with the same conditions as B up to an air with the same conditions of A, it is introduced the aerodynamic resistance $r_a \text{ (s/m)}$:

$$\lambda \cdot E_{B-A} = \frac{\rho \cdot c_p \cdot (T_A - T_B)}{r_a} \quad (2.5)$$

From point B to C, the mass of air increases its temperature, maintaining the saturated vapor pressure curve $e^o(T)$. Approximating the curve by the chord B-C with the slope Δ , the changes in the latent heat dQ_L and sensible heat dQ_S , result as it follows:

$$dQ = dQ_L + dQ_S = \frac{\lambda \cdot m \cdot 0.622}{p} \cdot de^o + m \cdot c_p \cdot dT; \quad (2.6)$$

$$dQ = \frac{\lambda \cdot m \cdot 0.622}{p} \cdot de^o + m \cdot \frac{\lambda \cdot 0.622 \cdot \gamma}{p} \cdot dT = \frac{\lambda \cdot m \cdot 0.622}{p} \cdot (de^o + \gamma \cdot dT) \quad (2.7)$$

$$dQ = \frac{\lambda \cdot m \cdot 0.622}{p} \cdot (\Delta \cdot dT + \gamma \cdot dT) = \frac{\lambda \cdot m \cdot 0.622}{p} \cdot (\Delta + \gamma) \cdot dT \quad (2.8)$$

Where Δ is the slope of the saturation vapor pressure-temperature curve de/dT .

Consequently, the proportions of dQ_L and dQ_S released from B to C, result:

$$\frac{dQ_L}{dQ} = \frac{\frac{\lambda \cdot m \cdot 0.622}{p} \cdot \Delta \cdot dT}{\frac{\lambda \cdot m \cdot 0.622}{p} \cdot (\Delta + \gamma) \cdot dT} = \frac{\Delta}{(\Delta + \gamma)} \quad (2.9)$$

$$\frac{dQ_S}{dQ} = \frac{\frac{\lambda \cdot m \cdot 0.622}{p} \cdot \gamma \cdot dT}{\frac{\lambda \cdot m \cdot 0.622}{p} \cdot (\Delta + \gamma) \cdot dT} = \frac{\gamma}{(\Delta + \gamma)} \quad (2.10)$$

Considering that the flow of heat received by the evaporating surface under the conditions of C is $R_n - G$, the water vapor diffusion occurring from the evaporating surface up to an air with the conditions of B would result:

$$\frac{\lambda \cdot E_{C-B}}{(R_n - G)} = \frac{\Delta}{(\Delta + \gamma)}; \quad \lambda \cdot E_{C-B} = \frac{\Delta}{(\Delta + \gamma)} \cdot (R_n - G) \quad (2.11)$$

By analogy to the path followed from B to A, the flux of latent heat from D to C would result:

$$\lambda \cdot E_{D-C} = - \frac{\rho \cdot c_p \cdot (T_C - T_D)}{r_a} \quad (2.12)$$

Consequently, the flux of latent heat released from D conditions ($T_D - e_D$) to A conditions ($T_A - e_A$), results:

$$\lambda \cdot E_{D-A} = \lambda \cdot (E_{B-A} + E_{C-B} + E_{D-C}); \quad (2.13)$$

$$\lambda \cdot E = \frac{\rho \cdot c_p \cdot [(T_A - T_B) - (T_C - T_D)]}{r_a} + \frac{\Delta}{(\Delta + \gamma)} \cdot (R_n - G) \quad (2.14)$$

Potential evaporation

Potential evaporation considers unlimited water supply in the evaporating surface, and the mass of air reaches saturated vapor pressure (in this case, point C and point D are the same):

$$\lambda \cdot E_P = \lambda \cdot (E_{B-A} + E_{C-B}) = \frac{\rho \cdot c_p \cdot (T_A - T_B)}{r_a} + \frac{\Delta}{(\Delta + \gamma)} \cdot (R_n - G) \quad (2.15)$$

And considering the following relationship (see Figure 2.4):

$$e_A^0 - e_A = (\Delta + \gamma) \cdot (T_A - T_B) \quad (2.16)$$

The Penman (1948) equation is obtained:

$$\lambda \cdot E_p = \frac{\Delta}{\Delta + \gamma} \cdot (R_n - G) + \frac{\rho \cdot c_p \cdot (e_A^0 - e_A)}{(\Delta + \gamma) \cdot r_a} \quad (2.17)$$

The original Penman (1948) equation distinguished two terms, one energetic term and one advective term dependent on the vapor pressure deficit and the diffusion of this vapor from the evaporating surface to the air.

$$\lambda \cdot E_p = \frac{\Delta}{\Delta + \gamma} \cdot (R_n - G) + \frac{\gamma}{\Delta + \gamma} \cdot \lambda \cdot E_a \quad (2.17b)$$

Where E_a is the advective term. To estimate the advective term, E_a , Penman initially proposed a Dalton-type expression $E_a = (e^0 - e) \cdot f(u)$, where $f(u)$ is an empirical expression as a function of wind speed u .

Nowadays, to characterize the water vapor transfer from the evaporating surface into the air, an aerodynamic resistance is considered:

$$r_a = \frac{\left[\ln \frac{z_v - d}{z_{0m}} \right] \cdot \left[\ln \frac{z_h - d}{z_{0h}} \right]}{k^2 \cdot u_z} \quad (2.18)$$

Where:

- z_v Height of wind speed measurements (about 2m)
- z_h Height of air humidity (about 2m)
- d Zero plane displacement of wind profile due to the presence of canopy
- z_{0m} Roughness length, momentum (height at which the speed is zero in the wind logarithmic profile)
- z_{0h} Roughness length, heat and water vapor (height at which the flow is zero in the heat and water vapor logarithmic profile)
- k Von Karman's constant (0.41)
- u_z Wind speed at z m above ground surface

Although the potential evaporation and potential evapotranspiration are many times applied equally, the diffusion of water vapor from the surface (stomata for the crops) to the air, when the evaporating surface is not a pan of water, is also subject to a specific surface resistance r_s .

Figure 2.5 Aerodynamic resistance r_a and total surface resistance r_s to water vapor flow.

Monteith (1965) modified the Penman equation to apply the study of vapor diffusion to the air from different crops, incorporating a representative resistance of the crop surface r_s to estimate potential crop evapotranspiration $\lambda \cdot ET_p$. The result was the Penman-Monteith equation, which presents a radiative term ($R_n - G$) and an advective term:

$$\lambda \cdot ET_p = \frac{\Delta(R_n - G) + \rho \cdot c_p \cdot \frac{(e^o - e)}{r_a}}{\Delta + \gamma \left(1 + \frac{r_s}{r_a} \right)} \quad (2.19)$$

Due to the lack of data to calculate the advective term in some occasions, approximation equations such as the Priestley-Taylor Method (Priestley and Taylor, 1972) have been proposed, which provides estimations of potential $\lambda \cdot E_p$ for no or low advective conditions by approaching the advection term of the Penman potential evaporation including a parameter $\alpha=1.26$.

$$\lambda \cdot E_p = \alpha_{PT} \cdot \frac{\Delta}{(\Delta + \gamma)} \cdot (R_n - G) \quad (2.20)$$

The Penman-Monteith equation is more theoretically accurate than other simplified approaches as the Priestley-Taylor Method, but requires resistance parameters that are difficult to characterize at global level. In this line, recent approaches have been developed to downscale potential Priestly-Taylor $\lambda \cdot ET_p$ values to actual $\lambda \cdot E$ based on plant physiological status and soil moisture availability (Fisher *et al.*, 2008).

Reference evapotranspiration

The Food and Agriculture Organization of the United Nations FAO, has recommended the Penman-Monteith equation for calculating the potential evapotranspiration of a reference evapotranspiring surface, completely shading the ground and never short of water. Reference evapotranspiration $\lambda \cdot ET_o$ is defined as the evaporative demand of the atmosphere for a reference evapotranspiring surface under the same conditions and can therefore be estimated from meteorological data alone, removing the influence of surface types in $\lambda \cdot ET_p$. According to Allen *et al.* (1998), this crop would correspond to an extensive area of grass (*alfa fescue*) of 12 cm height. FAO establishes a surface resistance $r_s = 70 \text{ s m}^{-1}$ for the reference crop when completely shaded and under well-watered conditions. In addition, certain approximations are assumed to calculate r_a , considering $h = 0.12 \text{ m}$, $d = 2/3 \text{ h}$; $z_{0m} = 0.123 \cdot h$ and $z_{0h} = 0.1 \cdot z_{0m}$. r_a would result $208/u_z \text{ (s m}^{-1}\text{)}$, where u_z is measured at 2m height. Adopting specific values of r_s and r_a for the reference crop, reference evapotarnspiration would result:

$$\lambda \cdot ET_o = \frac{\Delta \cdot (R_n - G) + \frac{\gamma \cdot 0.622 \cdot \lambda}{R_a \cdot T} \cdot u_z \cdot \frac{(e^0 - e)}{208}}{\Delta + \gamma \cdot \left(1 + u_z \cdot \frac{70}{208}\right)} \quad (2.21)$$

Where $R_a=0.287 \text{ kJ/kg/K}$ is the specific constant for dry air.

Dividing by λ , and considering that $1\text{MJ/m}^2/\text{day}=0.408 \text{ mm/day}$:

$$ET_o \text{ (mm/day)} = \frac{0.408 \cdot \Delta \cdot (R_n - G) + \gamma \frac{900}{T + 273} \cdot u_z \cdot (e^0 - e)}{\Delta + \gamma \cdot (1 + u_z \cdot \frac{70}{208})} \quad (2.22)$$

Crop evapotranspiration

Given the complexity in determining the specific resistances r_a and r_s for the calculation of the Penman-Monteith potential ET of a specific crop, Doorenbos and Pruitt (1977) established a methodology to estimate ET_p so that the ratio of ET_p to ET_o i.e. the crop coefficient K_c is:

$$ET_p = ET_o \cdot K_c \quad (2.23)$$

Actual evapotranspiration depends not only to the crop and the climate, but on the water content in the soil. Although the processes involved on ET are complex, certain approximations based on the water content in the soil are sometimes considered. As the water content in the soil decreases, the resistance of the stomata to the diffusion of water vapor into the air will be greater, and evapotranspiration will decrease. The reduction of evapotranspiration does not begin immediately after the soil dries, but when the crop has already evapotranspired the readily available moisture content RAM . When the soil water content is at field capacity, water is freely available and ET reaches potential values. When the soil water content reaches the wilting point, stomata completely close and $ET=0$.

Figure 2.6 Scheme of ET estimation as a function of soil moisture content.

ET in the agriculture fields has been traditionally estimated through the Doorenbos and Pruitt (1977) methodology. However, the real vegetative and growing conditions of the crop are approximated to those given by the K_c values, which poses uncertainties in the

estimations, particularly in water scarcity areas. Moreover, to assign specific K_c values among the different crop development stages and types over large heterogeneous areas is a difficult task, and the emergence of satellite-data allow to close this gap.

2.5 Measurements of evapotranspiration

For many applications, whether in hydrology, ecology or agriculture, direct measurements of H or λE are difficult, whether for practical, theoretical or economic reasons. Classic methods to estimate H or λE include lysimeters, Bowen ratio or Eddy Covariance.

Lysimeters are tanks filled with soil in which crops are grown under natural conditions to measure the amount of water lost by evaporation and transpiration (Jensen, 1990). In the Bowen Ratio, the energy balance is solved by measuring temperature ΔT and vapor pressure gradients Δe at two different heights above the evaporating surface to estimate β (Allen *et al.*, 2011):

$$\beta = \frac{H}{\lambda E} = \frac{\Delta Q_s}{\Delta Q_l} = \gamma \cdot \frac{\Delta T}{\Delta e} \quad (2.24)$$

Where γ is the psychrometric constant. Together with the measurement of net radiation R_n and sensible heat flux to the soil G , λE is solved by substituting β into the energy equation.

$$\lambda E = (R_n - G)/(1 + \beta) \quad (2.25)$$

The "Eddy covariance" technique solves λE based on the vertical analysis of instantaneous variations in wind speed and vapor density.

Figure 2.7 Eddy covariance scheme

Because of dealing with turbulent magnitudes, every variable is considered as the sum of a mean value ($\bar{x}$) plus a fluctuating term (x') according to the Reynolds decomposition $x = \bar{x} + x'$

Evaporation is equal to a mean product of the density for moist air (ρ_v) and vertical wind speed (v). Thus, the study of the water vapor transport in the atmosphere is expressed as:

$$\lambda E = \lambda \cdot \overline{v\rho_v} + \lambda \overline{v'\rho_v'} \quad (2.26)$$

Where mean vertical speed ($\bar{v}$) is assumed negligible for horizontal homogenous terrains.

$$\lambda E = \lambda \cdot \overline{v'\rho_v'} = \lambda \overline{(v - \bar{v}) \cdot (\rho_v - \bar{\rho}_v)} = \lambda \cdot cov[v, \rho_v] \quad (2.27)$$

2.6 State of the art on physical and empirical RS approaches to *ET* estimations

As an alternative to direct measurements, the estimation of *ET* by means of physical or empirical approaches has greatly evolved in recent years. As pointed out by Kalma *et al.* (2008), in the 1950s and 1960s the evaporation process was thought to be controlled largely by meteorological conditions, and much progress was conducted on local-scale evaporation processes. Since the 1980s, the study of the spatial variability of *ET* has gained a growing importance although there is still a paucity in the development of simulation models capable of estimating the distributed nature of land surface processes. Although point measurements with Eddy covariance or Bowen Ratio techniques have allowed to progress noticeably on the study of local evaporation processes, these measurements do not allow to measure *ET* at larger scales. The attraction of using remote sensing (RS) techniques to estimate evaporation at larger scales has emerged in the 1990s, providing economically sound observations of land surface temperature (*LST*) and other key variables to explain the partition of the surface energy balance. Surface energy balance (SEB) models are based on solving the surface energy balance equation introduced in this chapter, Eq. 2.1. Based on the physical principles of the evapotranspiration, the sensible heat (*H*) is estimated by the difference in temperature within the stomata of the leaves and the atmospheric layer surrounding the leaves, resulting:

$$H = \frac{\rho \cdot c_p \cdot (T_{aero} - T_a)}{r_a} \quad (2.28)$$

Where T_a is the temperature of the air at a specific height.

Where T_{aero} is the aerodynamic temperature of a surface, i.e that temperature which when combined with the air temperature and a resistance calculated from the log-profile

theory, provides an estimate of the surface sensible heat flux (Norman and Becker, 1995).

Simpler regression empirical models based on the relationships between λE and vegetation characteristics expressed through particular vegetation indices (VI) e.g. NDVI or EVI are sometimes comparable in accuracy to more complex SEB models, and present the overall advantage of being more simple and resilient in the presence of data gaps (Carter and Liang, 2018). Most of the application of these regression formulas, particularly in the agriculture field, are driven to the substitution of the crop coefficients by a RS-derived VI (Kalma *et al.*, 2008).

SEB models distinguish a wide range of approaches, including physical models that calculate λE as the residual of the SEB equation through thermal infrared data, and physical models that calculate λE directly based on combination equations.

In the residual approach, λE is solved indirectly as a residual of the SEB equation (Eq. 2.1). This approach include single-source models (“big-leaf” models), where the surface is considered homogeneous, and dual-source models, where the heat and mass fluxes from the soil and vegetation are computed separately. In the residual approach, thermal infrared data from RS (i.e. land surface temperature LST) are used to directly estimate sensible heat fluxes (H). These models have been widely used due to the advantage that they circumvent the estimation of the surface resistances r_s needed to compute λE (García *et al.*, 2013). In this approach, T_{aero} is substituted by the LST derived from the sensor in the calculation of H (Eq. 2.28). However, this substitution may lead to significant errors due to the difference between T_{aero} and LST , that reaches approximately 2°C and up to 10°C in partial vegetation covers (Kustas and Norman, 1996). Moreover, as a residual method, inaccuracies derived from the estimation of the other components of the SEB equation (i.e. R_n , G) may lead to accumulated errors in the final estimation of λE . The residual approach include models such as the RSEB (Kalma and Jupp, 1990), SEBAL (Bastiaanssen *et al.*, 1998a,b), SEBS (Su, 2002) or the triangle method (Nemani and Running, 1989).

Combination equations to directly estimate λE are mainly based on the Penman-Monteith (PM) equation (Eq.2.19). The main difficulties encountered to apply the PM equation lie on the characterization of the spatial and temporal variation of the surface resistances r_s for the diffusion of water vapor from the surface to the air without the use

of field data (García *et al.*, 2013). Simple approaches to estimate surface conductances include the use of prearranged parameters that rely on biome-type maps (Zhang *et al.*, 2010). One of the first attempts to characterize r_s through RS based on the PM approach was developed by Cleugh *et al.* (2007) after finding high biases when estimating λE by the residual approach in Australia. Alternatively, they used the PM approach assuming that soil evaporation was insignificant compared to transpiration from plants and therefore the surface resistance to evaporation r_s was equivalent to canopy resistance. They introduced an innovative aspect to calculate r_s by using a linear relationship based on the remote LAI vegetation index obtained from MODIS, with the premise that the greater the soil moisture and green canopy cover are, the larger is the signal in LAI . Thus, $G_s = C_L \cdot LAI + G_{smin}$, where G_s is the surface conductance (the inverse to the surface resistance r_s), which applies more correctly to canopy conductance, C_L is the mean stomatal conductance per unit LAI and G_{smin} is the surface conductance controlling the soil evaporation. As a consequence of obtaining inadequate results when testing the Cleugh's model against 19 AmeriFlux sites, Mu *et al.* (2007a) redefined the approach and developed the first RS-based global terrestrial ET map. In the Mu *et al.* (2007a) model, further improved in Mu *et al.* (2011), a separate term for soil evaporation is included. In this approach potential soil evaporation $\lambda E_{soil_{pot}}$ is constrained by a soil moisture function taken from Fisher *et al.* (2008) which relies on the complementary hypothesis stated by Bouchet (1963) on the land-atmosphere interactions of VPD and relative humidity (%), $(RH/100)^{VPD/200}$. In addition, Mu *et al.* (2007a) improved the canopy conductance calculations of the Cleugh's model by considering two functions that account for the response of the stomata to VPD and temperature (T). The canopy conductance for transpiration G_c is up-scaled from stomatal conductance C_s up to the canopy level by means of LAI (Mu *et al.*, 2013). Thus, $G_c = C_s \cdot LAI$ where $C_s = C_L \cdot m(T_{min}) \cdot m(VPD)$ and C_L is the mean potential stomatal conductance per unit leaf area. A map of vegetation types in combination with a biome properties lookup table is provided in this model to define the T_{min} and VPD -depending functions. Alternatively to the earlier empirical models of G_s in Cleugh *et al.* (2007) and G_c in Mu *et al.* (2007a), Leuning *et al.* (2008) proposed a biophysical algorithm to calculate G_c , reformulating the Kelliher *et al.* (1995) approach by including the effect of VPD and light response on stomatal conductance. This approach requires a two-parameter optimization, the maximum stomatal conductance of leaves g_{sx} and a soil

evaporation factor f . The consideration of the model parameters as fix along the year result low performances of λE estimations at drier sites (García *et al.*, 2013). This is mainly due to the overestimation of λE in some semiarid and arid catchments due to non-restrictions to the water balance in the application of the Leuning model (Zhang *et al.*, 2010). To circumvent this issue, (Zhang *et al.* (2008); Zhang *et al.*, 2010) improved the performance of the Leuning model by considering f as a soil moisture variable dependent on precipitation for each grid cell. Also, they optimized the value of g_{sx} by forcing λE estimated from a hydrological model to λE derived from the Leuning model (Zhang *et al.*, 2010). The results were still poor in drier sites as compared to humid sites (García *et al.*, 2013).

The recent trends on λE estimations have evolved towards increasing complexity as opposed to applicability (Fisher *et al.*, 2008). Although the PM approach is more theoretically accurate than other simpler approaches as the Priestley Taylor (PT) equation, the parameters and inputs needed, limit its application in areas where data availability is scarce, and sometimes the uncertainties derived from the estimation of the parameters required may lead to higher errors in its application. To overcome the difficulties derived for the characterization of the spatial and temporal variation of surface resistances in the PM approach, the PT equation (Priestley and Taylor, 1972) proposes the replacement of these resistances by an empirical multiplier α_{PT} (Eq. 2.20). Fisher *et al.* (2008) proposed a RS PT-based model, the PT-JPL model, in which the potential evapotranspiration remains as in the original formulation. To estimate actual values of evapotranspiration, they include a novelty in the approach, in which potential λE is downscale to actual values based on series of soil and canopy ecophysiological constraints to evapotranspiration. This model results very attractive due to its simplicity for application and potentiality for regionalization, and although proved to be successful over 36 Fluxnet sites, none of them included semiarid vegetation (García *et al.*, 2013).

Although RS combination approaches based on either PM or PT have taken advantage of remotely-sensed derived data from the optical region, the use of thermal infrared data had not received much attention. Contrary to the soil moisture constraint considered in the Fisher *et al.* (2008) and in the Mu *et al.* (2011) approaches, based on the complementary hypothesis stated by Bouchet (1963), García *et al.* (2013) proposed an adaptation to the PT-JPL model by introducing a new formulation for soil moisture

based on the apparent thermal inertia concept ATI , which has proved to perform well at point-scale EC flux sites with scarce availability of water.

CHAPTER 3

Methodology

3 Methodology

3.1 Study area

3.1.1 Doñana region and surrounding irrigated areas

The Doñana region, which extends over about 290000 ha, is located in south-western Spain, including several territories under different environmental protection: the Doñana National Park, the Doñana Natural Park and the UNESCO Biosphere Reserve. The availability of water is crucial in the area and represents the limiting factor for the sustainability of the aquatic and terrestrial ecosystems. The water availability in the region relies on different sources: a system of regional streams, the Almonte-Marismas aquifer and the rainfall.

The surrounding irrigated areas on the left bank of the River are part of the ancient Guadalquivir marshes, where 74400 ha of marshlands were transformed into arable lands in the 1960s through the “Irrigation Area of the Lower Guadalquivir” project (Martín-López *et al.*, 2011), amongst them the BXII Irrigation District.

Figure 3.1 Map of the UNESCO protected study area, including (i) irrigated areas: mixed-irrigation areas (BXII and left bank) and rice fields; (ii) natural ecosystems: wetland, shrubland and coniferous forest in the Doñana National Park.

3.1.2 BXII Irrigation District

The BXII Irrigation District covers an area of 15000 hectares near the Atlantic coast of South-West Spain, close to the estuary of the Guadalquivir River within the ancient Guadalquivir marshes surrounding the Doñana region (See Fig. 3.1). Aiming to the development of agriculture in the area, a soil reclamation project was conducted in the second half of the XX century, representing nowadays the main economic activity in the region. As drainage was almost non-existent in natural conditions, tile drainage systems were gradually installed, and after decades of salt leaching, a project of irrigation was set up in the 1970s (Fig. 3.2)

Figure 3.2 BXII Irrigation District, scheme of the irrigation and drainage systems

3.2 Hydrological modelling using a conceptual semi-distributed model

As an approximation to the hydrological study of the BXII Irrigation District, the conceptual hydrological model WATEN was developed. Series of drainage, soil moisture deficit and evapotranspiration (ET) were determined from precipitation, reference evapotranspiration and irrigation. These variables are interrelated and require iterative calculation for their resolution. We have calibrated the model using the energy consumption data in the drainage pumping stations. The traditionally applied SOLVER algorithm alone is not powerful enough to find, in all cases, a single solution that optimizes the chosen objective function. Methods based on "multistart" procedures, which calculate local minimums and then select the absolute minimum value among

them, were introduced in WATEN calibration. In addition, and given that practical experience shows that model calibration focused on a single objective function may not give adequate results, multi-objective optimization was conducted. Considering the “equifinality problem” that points to the existence of several parametric vectors that may work reasonably well, we used robust approaches for its estimation. We implemented a method we named PEDT (Parameters Estimation based on Driven Trials). Following this method, we run a number of 40000 simulations with randomly estimated parameters following uniform distributions. Although, due to the number of Markov Chain Monte Carlo simulations computed, this method required more computing time than classical methods to determine the optimal model parametric vectors, it allowed choosing the final set of parametric vectors that reached better indexes for the considered objective-functions.

While a reduced number of parameters define the semi-distributed model WATEN developed in this study, the spatial distribution of the model parameters would require a more complex calibration that could result in a model over-parameterization. Satellite data offers promising opportunities to discriminate models components at spatio-temporal scales overcoming this issue.

3.3 Surface energy balance modelling to estimate evapotranspiration at spatio-temporal scales

A series of global observations were acquired from the Moderate Resolution Imaging Spectroradiometer (MODIS), using sensors from both Aqua and Terra satellites. Satellite data was used in combination with climatic data: air temperature and radiation, in order to run the spatialized thermal version of the PT-JPL model. MODIS land products were retrieved from The Earth Observing System Data and Information System (EOSDIS), a core capability in National Aeronautics Space Administration (NASA) Earth Science Data Systems Program. All the selected MODIS products were acquired at 1km pixel resolution during a chrono-sequence spanning from 2003-2016. The temporal resolution of the data sets varied from 8-day-composites of Leaf Area Index (LAI) and Fraction of Photosynthetically Active Radiation (f_{APAR}) from MOD15A2; 8-day-composites broadband surface albedo (α) acquired from MCD43B3; 16-day-composites of Normalized Difference Vegetation Index ($NDVI$) retrieved from MOD13A2 and daily Land Surface Temperature (LST) and Emissivity ($Emis$) from MOD11A2 and MYD11A2.

In this work, the Priestley-Taylor Jet Propulsion Laboratory model, PT-JPL (Fisher *et al.*, 2008) was spatially distributed over the thermal-version developed by García *et al.* (2013). This version introduces a soil moisture formulation based on the thermal inertia concept. The PT-JPL model retrieves actual evapotranspiration (λE) -latent flux in energy terms-, from combining actual canopy transpiration (λE_c) and soil evaporation (λE_s) (Eq. 3.1). The quantity of water intercepted by the canopy was not considered in the formulation of the model (García *et al.*, 2013) due to the low density of vegetation cover.

$$\lambda E = \lambda E_c + \lambda E_s \quad (3.1)$$

To formulate λE , the model starts from potential crop evapotranspiration λEp . It establishes a reduction from both the potential transpiration from the canopy (λEp_c) and the potential evaporation from the soil (λEp_s) considering biophysical limitations from the canopy ($biolim_c$) and the soil ($biolim_s$) (García *et al.*, 2013) (Eq. 3.2).

$$\lambda E = \lambda Ep_c \cdot biolim_c + \lambda Ep_s \cdot biolim_s \quad (3.2)$$

3.3.1 Canopy transpiration

Actual canopy transpiration (λE_c) results from adjusting λEp_c to its actual value by considering different plant physiological constraints: the fractional area of the canopy actively transpiring (f_g), a plant moisture constraint (f_m) and a plant temperature factor (f_t) (Eq. 3.3).

$$\lambda E_c = \lambda Ep_c \cdot f_g \cdot f_m \cdot f_t \quad (3.3)$$

The potential canopy evapotranspiration λEp_c is based on Priestley-Taylor (Eq. 3.4):

$$\lambda Ep_c = \alpha_{PT} \cdot \frac{\Delta}{\Delta + \gamma} \cdot (R_{nc} - G) \quad (3.4)$$

Where α_{PT} is the Priestley-Taylor coefficient (1.26 $\text{kPa } ^\circ\text{C}^{-1}$); Δ is the slope of the vapor pressure curve ($\text{Pa } ^\circ\text{K}^{-1}$) which depends on the mean temperature of the day (K); γ is the psychrometric constant, which depends on the atmospheric pressure at considered elevation; R_{nc} is the daily net radiation from the canopy (Wm^{-2}) further calculated as ($R_n - R_{ns}$) and G is the soil heat flux (Wm^{-2}) considered minimal in this study (Fisher *et al.*, 2008).

R_n at the land surface is expressed in terms of shortwave (R_S) and longwave (R_L) radiation components (Eq. 3.5).

$$R_n = R_L^\downarrow - R_L^\uparrow + R_S^\downarrow - R_S^\uparrow = R_L + R_S \quad (3.5)$$

Where $R_L^\downarrow$ and $R_L^\uparrow$ are the incoming and outgoing longwave radiation components (Wm^{-2}), $R_S^\downarrow$ and $R_S^\uparrow$ are the incoming and outgoing shortwave radiation components (Wm^{-2}) (Bisht *et al.*, 2005).

Incoming longwave radiation $R_L^\downarrow$

To calculate instantaneous $R_L^\downarrow$, we followed Idso and Jackson (1969) (Eq. 3.6).

$$R_{L_{inst}}^\downarrow = \sigma \cdot (T_{air_{MODIS-time}} + 273.15)^4 \cdot \left[1 - \left(c \cdot e^{\left(-d \left(T_{air_{MODIS-time}}^2 \right) \right)} \right) \right] \quad (3.6)$$

Where σ is the Stefan-Boltzmann constant ($5.67 \times 10^{-8} \text{ Wm}^{-2}$), c and d are constants (0.261 and 7.77×10^{-4} respectively), $T_{air_{MODIS-time}}$ ($^{\circ}\text{C}$) is the air temperature at the time of MODIS overpass, calculated as in Parton and Logan (1981) (Eq. 3.7).

$$T_{air_{MODIS-time}} = (T_{max} - T_{min}) \cdot \sin\left(\frac{\pi \cdot m}{N + 2 \cdot d}\right) + T_{min} \quad (3.7)$$

Where T_{max} and T_{min} ($^{\circ}\text{C}$) are acquired from the agro-climatic station Lebrija I (IFAPA, 2014), N (h) is the time elapsed between sunrise and sunset, from NOAA Sunrise/Sunset and Solar Position Calculators, d is the time lag coefficient for the maximum temperature before sunset (1.86 h), m is the number of hours after the minimum temperature occurs until sunset (Parton and Logan, 1981) (Eq. 3.8).

$$m = MODIS_{time} - \left(12 - \left(\frac{N}{2} \right) + c \right) \quad (3.8)$$

Where $MODIS_{time}$ was extracted from MYD11A2, as a mean value in the study area, c is the time lag in minimum air temperature after sunrise (-0.17 h).

Outgoing longwave radiation $R_L^\uparrow$

The outgoing longwave instantaneous radiation was calculated at the time of MODIS overpass time, following García *et al.* (2007) (Eq. 3.9).

$$R_{L_{inst}}^\uparrow = -\varepsilon_S \cdot \sigma \cdot T_S^4 \quad (3.9)$$

Where ε_S is an average of the emissivity bands 31 and 32, T_S is the Land Surface Temperature, acquired from MYD11A2.

Shortwave radiation R_S

To retrieve daily shortwave radiation (Wm^{-2}), we formulated (Eq. 3.10):

$$R_{S_{day}} = R_{S_{day}}^{\downarrow} \cdot (1 - \alpha) \quad (3.10)$$

$R_{S_{day}}^{\downarrow}$ ($\text{MJ/m}^2/\text{day}$) was acquired from the agro-climatic station Lebrija I (IFAPA, 2014); α is the broadband surface albedo, considering the 16-days Terra data derived from the combined product MCD43B3. We assumed that diffuse radiation is a 20% of the total incoming radiation. Albedo was formulated by combining broadband black and white-sky-albedo as in (Eq. 3.11) (Rasmussen *et al.*, 2014).

$$\alpha = 0.8 \cdot \alpha_{BSA} + 0.2 \cdot \alpha_{WSA} \quad (3.11)$$

Net radiation

To obtain daily net radiation R_n , R_L and R_S were computed on daily terms. We first converted $R_{S_{day}}$ into $R_{S_{inst}}$ (Eq. 3.12) using a conversion factor J (Eq. 3.13). This equation was adjusted from Jackson *et al.* (1983) in order to maintain the same units of time (h) in both N and t , thus avoiding imbalance in the equation.

$$R_{S_{inst}} = \frac{R_{S_{day}}}{J} \cdot \frac{24}{N} \quad (3.12)$$

$$\text{Where } J = \frac{2}{\sin\left(\frac{\pi t}{N}\right)} \quad (3.13)$$

Where N (h) is the time elapsed between sunrise and sunset, retrieved from NOAA Sunrise/Sunset and Solar Position Calculators (NOAA), t (h) is the time elapsed between the sunrise time obtained from NOAA and $MODIS_{time}$.

Thereafter, $R_{S_{inst}}$ was aggregated to $R_{L_{inst}}$ (Eq. 3.14) to be then converted into daily net radiation R_n (Eq. 3.15) by applying the conversion factor J (Eq. 3.13).

$$R_{n_{inst}} = R_{L_{inst}} + R_{S_{inst}} \quad (3.14)$$

$$R_n = R_{n_{inst}} \cdot J \cdot \frac{N}{24} \quad (3.15)$$

R_n is partitioned into net radiation from the soil R_{n_s} (Eq. 3.16) and net radiation from the canopy R_{n_c} (Eq. 3.17) following Norman *et al.* (1995) and García *et al.* (2013).

$$R_{n_s} = R_n \cdot e^{(-k_{Rn} \cdot LAI)} \quad (3.16)$$

Where $k_{Rn} = 0.6$ (Impens and Lemeur, 1969; García *et al.*, 2013), LAI is the Leaf Area Index retrieved from 8-day-composites MOD15A2.

$$R_{n_c} = R_n - R_{n_s} \quad (3.17)$$

Biophysical limitations to the canopy

The green canopy fraction (f_g) is the ratio between absorbed (f_{APAR}) and intercepted (f_{IPAR}) photosynthetically active radiation (PAR) -solar radiation in the 0.4-0.7 μm range- by vegetation canopy (Eq. 3.18).

$$f_g = f_{APAR} / f_{IPAR} \quad (3.18)$$

Where f_{APAR} was acquired from the 8-day-composite MOD15A2. It is determined as a linear function of the Enhanced Vegetation Index (EVI) (Gao *et al.*, 2000); (Xiao *et al.*, 2004); (Zhang *et al.*, 2005). It can also be derived from the Soil Adjusted Vegetation Index ($SAVI$) when the information on blue reflectance is not available (Fisher *et al.*, 2008), f_{IPAR} accounts for the fraction of PAR intercepted by the vegetation cover, generally estimated as a function of the Normalized Difference Vegetation Index ($NDVI$) (Zhang, 2005; (Fisher *et al.*, 2008) (Eq. 3.19).

$$f_{IPAR} = m_2 \cdot NDVI + c_2 \quad (3.19)$$

Where $NDVI$ was acquired from the 16-day-composites MOD13A2, $m_2 = 1$, $c_2 = -0.05$.

The plant moisture constraint (f_m) considers a reduction on the efficiency of potential light utilization in response to the effects of water stress (Potter *et al.*, 1993; Fisher *et al.*, 2008) (Eq. 3.20).

$$f_m = \frac{f_{APAR}}{f_{APARmax}} \quad (3.20)$$

The plant physiological limitation (f_l) accounts for an efficiency reduction on light absorption from plants when they are exposed to temperature ranges far away their optimum (Potter *et al.*, 1993). García *et al.* (2013) implements the Carnegie-Ames-Stanford Approach model ($CASA$) developed by Potter *et al.* (1993) where f_l depends on T_{opt} ($^{\circ}C$) and mean daily air temperature Ta_m ($^{\circ}C$). It captures the behaviour of variations on light utilization efficiency as an asymmetric bell that falls off more quickly at higher temperatures (Eq. 3.21).

$$f_t = 1.1814 / [(1 + e^{0.2 \cdot (T_{opt} - 10 - Ta_m)})] / [(1 + e^{0.3 \cdot (-T_{opt} - 10 + Ta_m)})] \quad (3.21)$$

The optimum air temperature T_{opt} (°C) for plant development was fixed at 25 °C as in broadly-applied modelling approaches (Yuan *et al.*, 2010) and suggested as close to optimum in the site. In preliminary analyses conducted by García *et al.* (2013), the model was not significantly sensitive to temperature variations of $\pm 5^\circ\text{C}$ to this value. Ta_m (°C) was acquired from the agro-climatic station Lebrija I (IFAPA, 2014).

3.3.2 Soil evaporation

Potential soil evaporation λEp_s was reduced by considering a soil moisture constraint (f_{sm}) dependent on soil water content (García *et al.*, 2013) (Eq. 3.22).

$$\lambda E_s = \lambda Ep_s \cdot f_{sm} \quad (3.22)$$

$$\text{Where } \lambda Ep_s = \alpha_{PT} \cdot \frac{\Delta}{\Delta + \gamma} \cdot (R_{ns} - G) \quad (3.23)$$

Where G is the soil heat flux, considered minimal in this study (Fisher *et al.*, 2008).

The soil moisture constraint f_{sm} relies on the concept of thermal inertia (TI). Thermal inertia represents the ability of a material to conduct heat, described as the land surface resistance to temperature oscillations. TI can be an indicative of soil moisture content (SMC) variations (Peters *et al.*, 2011). Soil TI increases with increments in the soil water content. Higher soil water content results on lower diurnal temperature oscillations. A simple approximation to this concept is the apparent thermal inertia (ATI) derived from multi-spectral remote sensing images (Mitra and Majumdar, 2004); (Verstraeten *et al.*, 2006). The aforesaid ATI (Eq. 3.24) results from combining surface albedo α , maximum land surface temperature oscillations ($LST_{Day} - LST_{Night}$), and a solar correction factor C .

$$ATI = C \cdot \frac{1 - \alpha}{(LST_{Day} - LST_{Night})} \quad (3.24)$$

Where α is the broadband surface albedo acquired from MCD43B3, formulated as in Eq. 3.11, ($LST_{Day} - LST_{Night}$) accounts for the maximum land surface temperature oscillations per day. For its formulation, the maximum and minimum values of LST from MOD11A2 and MYD11A2 were selected, C is the solar flux variation at latitude θ and solar declination factor ϕ that results from the method developed by Iqbal (1983) (Eq. 3.25).

$$C = \sin\vartheta \cdot \sin\varphi \cdot (1 - \tan^2\vartheta \cdot \tan^2\varphi) + \cos\vartheta \cdot \cos\varphi \cdot \arccos(-\tan\vartheta \cdot \tan\varphi) \quad (3.25)$$

Cloudy meteorological conditions at satellite overpass time blocked the thermal and solar wavelengths, hindering the acquirement of daily *LST* data (Qin *et al.*, 2013). Therefore, in this study *ATI* was acquired from 8-day *LST* data composites. *ATI* accounts for canopy and soil spatio-temporal water content variations (Verstraeten *et al.*, 2006) although the coupling is not straightforward (García *et al.*, 2013). The formulation of *ATI* relies on the minimum and maximum seasonal *ATI*, respectively. Assuming that maximum *ATI* values occur at saturated soil moisture content conditions and that minimum *ATI* corresponds to the residual soil water content in the soil, f_{sm} would approximate the difference between actual water content and field capacity (Verstraeten *et al.*, 2006) (Eq. 3.26).

$$f_{sm} = \frac{ATI - ATI_{min}}{ATI_{max} - ATI_{min}} \quad (3.26)$$

CHAPTER 4

Results

4 Results

4.1 Study I. Water balance and flow rate discharge on a receiving water body: application to the BXII Irrigation District in Spain

Abstract. The quantification of the main water balance components becomes necessary to diminish the pollutants load from drainage, and its harmful effect on the environment, aggravated within a context of increasing water scarcity. As a first approach to the hydrological study of the 15000 ha BXII Irrigation District in Spain, a conceptual lumped model entitled WATEN has been developed, aiming to calculate the monthly flow rate discharge to the Guadalquivir River over the period 2002-2012. The model requires as inputs, irrigation, precipitation and potential crop evapotranspiration. Main model parameters are the total and readily available moisture in the soil, the effective rainfall and the irrigation efficiency. Energy consumption for drainage discharge was used for calibration. Both classical optimization and a robust approach based on Monte Carlo were performed. To diminish computational requirements, Monte Carlo was not haphazardly applied, but conducted on a similar manner to genetic algorithms, entitled Parameters Estimation on Driven Trials (PEDT). The model attained an average Nash-Sutcliffe coefficient $e_2 \cong 0.90$ between observed and estimated drainage discharge. It was noted a significant crop evapotranspiration reduction compared to potential values. Furthermore, the volume of water discharged to the river might be sufficient for leaching irrigation water salts.

4.1.1 Introduction and objectives

Irrigated agriculture reinforces land productivity and crop diversity, particularly in arid and semiarid areas (Tanji and Kielen, 2002). However, intensive agriculture at catchment scale, directly impacts on downstream water bodies (Steduto *et al.*, 2012). To diminish the negative effects, the European Water Framework Directive (WFD, 2000) pursues an integral approach in terms of water quality and quantity allocation.

Irrigated agriculture is the largest water consumer, accounting for 70 percent of freshwater withdrawals (WWAP, 2012). The increasing global water demand is aggravating the competition between agriculture and the environment for fresh and good quality water. Drainage water, containing agrochemicals and salts, may degrade water quality in receiving water bodies (Ongley, 1996), intensifying water scarcity,

especially where regulations are slightly enforced (Steduto *et al.*, 2012). It is predicted that climate change will worsen this situation (Turral *et al.*, 2011).

Climate change may aggravate water scarcity in the Mediterranean basin (Field, 2012), affecting crop productivity in the coming decades (Tubiello and van der Velde, 2010). Irrigated agriculture has been practised for millennia in the Guadalquivir river basin (Spain), rising by 500% since 1900. This tendency, mostly pronounced over the last decade, has led to the reduction of the assigned water per irrigation district (Rodríguez-Díaz *et al.*, 2007).

The BXII Irrigation District of the Lower Guadalquivir Irrigated Area (BXII ID) is one of the largest irrigated areas in Spain. It is referred to as a nitrate vulnerable zone (CHG, 2013) following the European Commission nitrates directive (EU, 1991). As pointed out by Barros *et al.* (2011), the management and quantification of water balances becomes necessary to diminish the pollutants load from drainage and its harmful effect on the environment, particularly at irrigation district scales. On this line, the European Commission has joined forces to elaborate physical water balances models at basin levels (EU, 2014). Experience has shown that water balances often need to be implemented at different stages, including extended information as needs arise (Steduto *et al.*, 2012).

The lack of robust data is a restrictive factor when it comes to conduct complex or physically based models (Wagener *et al.*, 2003). When not enough data is available, the successful application of a conceptual rainfall-runoff model (CRR), in particular rainfall-runoff flow in this study, depends on the accuracy of calibration (Diskin and Simon, 1977).

Classical calibration research has been based on mathematical optimizations of either single or multi-objective functions. The complexity of finding a unique set of parameters to optimize a CRR model has been historically reported. Numerous studies have relied on the improvement and comparison of optimization algorithms (e.g., Duan *et al.*, 1992; Yapo *et al.*, 1998; Vrugt *et al.*, 2003; Kollat and Reed, 2006; Skahill and Doherty, 2006). The considered objective function often presents local minima, which do not guarantee to find the optimized parametric vector. (Beven and Freer, 2001) pointed to numerous model structures and parameters vectors which may reasonably approach observed data. Robust parameter optimization is an alternative to classical optimization (Bárdossy and Singh, 2008). It is no longer based on algorithms which

optimise objective functions, but on a geometric Monte Carlo simulations process search for robust parametric vectors (Cullmann *et al.*, 2011). It has been widely applied in successful applications (e.g., Seibert, 1999; Choi and Beven, 2007; Rientjes *et al.*, 2013).

In this study, we have developed a conceptual hydrological model WATEN, aiming to calculate the flow rate discharged from the BXII ID to the Guadalquivir River over the period 2002-2012. The aim of this work is to approach the hydrological study of an Irrigation District lacking of robust data in such a manner that the water balance is performed from less to more process complexity.

The present study is intended to be the basis for similar worldwide studies, and to serve as a guide for future alike applications. The characteristics of the BXII ID are analogous to many others coastal irrigation districts with drainage discharge to receiving water bodies, as is the case of many irrigated areas of Egypt, Pakistan or India amongst others (Ritzema, 2009).

4.1.2 Study area

The BXII ID covers an area of about 15000 hectares. It is part of the Guadalquivir Marshland, located near the Atlantic coast of South-West Spain, close to the estuary of the Guadalquivir River (Figure 1).

Figure 4.1 Location and aerial view of the BXII Irrigation District of the Lower Guadalquivir Irrigated Area.

A soil reclamation project was conducted in the second half of the XX century. After decades of salt leaching, irrigation was set up over the 1980s and nowadays, agriculture represents the main economic activity in the area.

For the irrigation system, three secondary canals receive water from Melendo reservoir. Water is pumped and distributed to the fields through sprinklers, furrow or drip irrigation. A system of subsurface drainage controls the groundwater table and permits the leaching of salts. From the fields drainage flows into progressively larger drainage canals, which dispose the effluent to the river through a system of tidal gates and pumping stations. Tidal gates are only used at occasional peak water levels.

4.1.3 Methodology

4.1.3.1 Data availability

Monthly data of land use, precipitation, irrigation and energy consumption at drainage pumping stations has been accessible for the period 2002-2012.

Percentages of land use for major crops are: cotton, 38% from 20/4 to 27/9; beet, 34% from 1/11 to 9/06; tomato 10%, 1/04 to 20/07; wheat, 5%, from 10/11 to 9/05; corn, 4%, 10/03 to 7/08; sunflower, 3%, 10/03 to 18/08 and others, 6%.

Daily precipitation data (P) is available from the agro-climatic station Lebrija I (IFAPA, 2014).

Irrigation data (I) was estimated based on monthly irrigation water allocated to Melendo by the Guadalquivir Hydrographic Confederation, CHG. Melendo reservoir presents a permanent regime of water entries and discharges to the BXII ID over summer months, which do not apply in winter. For data verification, irrigation water allocated to Melendo was compared with flowmeters data (Mateos, personal communication) installed on the irrigation canals over the period 2008-2011. Compared data series showed significant monthly differences, reduced to a 2.5% discrepancy in terms of cumulative monthly data. Data from Melendo attained slightly higher total values and showed a certain delay over spring time: when irrigation is applied, the reservoir gets gradually emptied and is replenished over summer time. The month of March may present some inconsistencies, and the corresponding values might be greater than reservoir records (Figure 4.2).

Figure 4.2 Average monthly irrigation data from Melendo reservoir logs and canals flowmeters data over the period 2008-2011.

Potential crop evapotranspiration (ET_P) was calculated as $ET_P = ET_o \cdot K_c$, where reference evapotranspiration (ET_o) is supplied by the agro-climatic station Lebrija I (IFAPA, 2014). The estimation of crop evapotranspiration might over or under predict its real value. Farahani *et al.* (2008) warned about the blind application of Allen *et al.* (1998) methodology and different authors argued the necessity of regionalising crop coefficient values (Piccinni *et al.*, 2009; Bezerra *et al.*, 2012). For this study, crop coefficient values (K_c) were obtained by consulting CROPWAT database (FAO, 2013). Specific basal crop coefficient values (K_{cb}) were supplied by the Guadalquivir Hydrographic Confederation, (CHG, 2005), table 4.1.

Table 4.1 Crop coefficients K_{cb} , lengths of crop development stages (L_{ini} , L_{dev} , L_{mid} , L_{end}) and initial and final date of crop development stages (f_o , f_4) (CHG, 2005).

Crop	Beetroot	Wheat	Cotton	Tomato	Corn	Sunflower
Crop coefficients						
K_{cb1}	0.15	0.15	0.15	0.15	0.15	0.15
K_{cb2}	1.05	1.1	1.13	1.15	1.15	1.05
K_{cb3}	0.55	0.15	0.3	0.7	0.45	0.25
Lengths of crop development stages (days)						
L_{ini}	60	30	30	20	30	20
L_{dev}	80	50	50	40	40	40
L_{mid}	90	70	50	40	50	50
L_{end}	20	30	30	10	30	20
Initial and final date of crop development stages						
f_o	01-Nov	10-Nov	20-Apr	01-Apr	10-Mar	10-Mar
f_4	09-Jul	09-May	27-Sep	20-Jul	07-Aug	18-Jul

No flowmeters are installed to quantify the volume of water discharged to the river. Drainage (D) has been calculated from energy consumption data at the six drainage pumping stations: pumping groups are models H-530 and H-800 (Figure 4.3).

Figure 4.3 Pump performance curves derived from manufacturer information for pumping groups H-530 and H-800, and energy consumption per unit volume (E_u).

Model H-530 turns on at first place followed by one or two pumping groups H-800 when necessary. Lengths, diameters, geometric heads and pumps suction and impulsion capabilities were measured. It served to propose certain work hypotheses and corroborate conversion values (E_u) between energy consumption, E , and drainage, D . Drainage pumping stations Señuela and Tarfia reached together 76.8% energy consumption. Pump geometric heights range from 3 to 4.7 m in Señuela and from 2.45 to 5.1 m in Tarfia. Fig. 4.4 represents energy consumption per unit volume, E_u , at every geometric height (Δz). It was assumed that pumping groups were designed to work at nominal flow conditions, and at a project geometric height $\Delta z_p = 4.25$ m.

Figure 4.4 Estimation of energy consumption per unit volume (E_u) as function of geometric height (Δz).

The E_u value of Model H-800 is $2.5 \text{ W}\cdot\text{h}/\text{m}^3$ lower than the corresponding to model H-530. An intermediate E_u value might apply for the whole system.

4.1.3.2 Model equations and parameters

A simplified scheme of the water balance is represented in Figure 4.5. Subsurface drains are placed at one-meter depth and ten-meters distance, reduced to 5 meters in some occasions. Soil structure is compacted underneath 70 cm, not allowing deep filtrations. Loose material above the drains permits the conduction of water.

Figure 4.5 Water balance scheme in the BXII ID.

4.1.3.2.1 Model equations

For hydrological modelling of the catchment, we developed a volumetric model: WATEN. Series of actual crop evapotranspiration, ET , drainage, D , and soil moisture variation, $S-S_{i-1}$, were determined based on precipitation, P , irrigation, I , and reference evapotranspiration, ET_o , data, Eq. (4.1):

$$P + I = ET + D + S - S_{i-1} \quad (4.1)$$

When there is sufficient water, ET reaches its potential value ET_p , otherwise, it is unknown. On this line, programmes like CROPWAT (FAO, 2013) utilise concepts such as soil moisture depletion (SMD), readily available moisture (RAM), and total available moisture (TAM) in the soil. SMD is expressed as $SMD = S_M - S$, where S_M is the maximum value of soil moisture, S . S_M is equivalent to TAM and RAM is defined as $RAM = p \cdot TAM$, where p , provided by CROPWAT (FAO, 2013), is the mean fraction of TAM used up from the root zone before water stress occurs.

WATEN resolves Eq. (4.2), (4.3) and (4.4) for ET , D and SMD resolution. Logical variables are implemented (indicated in smaller letter format in the Equations) taking a value 1 when true and 0 when false. This manner, each equation can be introduced as a unique sentence in an Excel spreadsheet or Matlab script. These equations are interrelated, and require of iterative calculation for its resolution.

$$ET = \begin{cases} ET_p & \cdot (SMD \leq RAM) + \\ ET_p \cdot \frac{TAM - SMD}{TAM - RAM} & \cdot (SMD > RAM) \end{cases} \quad (4.2)$$

A fraction of precipitation (R_p) and irrigation (R_I) is effective. Complementary fractions, $1-R_p$ and $1-R_I$, respectively, are lost by drainage.

$$SMD = \begin{cases} (SMD_{i-1} + ET - P \cdot R_p - I \cdot R_I) & \cdot (0 < SMD_{i-1} + ET - P \cdot R_p - I \cdot R_I < TAM) + \\ TAM & \cdot (SMD_{i-1} + ET - P \cdot R_p - I \cdot R_I > TAM) \end{cases} \quad (4.3)$$

$$D = \begin{cases} P \cdot (1 - R_p) + I \cdot (1 - R_I) & + \\ (P \cdot R_p + I \cdot R_I - SMD_{i-1} - ET) & \cdot (P \cdot R_p + I \cdot R_I - SMD_{i-1} - ET > 0) \end{cases} \quad (4.4)$$

Where the subscript ($i-1$) refers to the preceding month.

Eq. (4.3b) has been derived from Eq. (4.2) and Eq. (4.3) in order to reduce computational time. It permits to obtain SMD without iterative calculations.

$$SMD = \begin{cases} ASMD & \cdot (0 < ASMD < RAM) + \\ \left(ASMD - \frac{ET_p \cdot (ASMD - RAM)}{TAM - RAM + ET_p} \right) & \cdot (RAM < ASMD < TAM + ET_p) + \\ TAM & \cdot (ASMD > TAM + ET_p) \end{cases} \quad (4.3b)$$

Where $ASMD = SMD_{i-1} + ET_p - P \cdot R_p - I \cdot R_I$ (Figure 4.6):

Figure 4.6 Soil moisture depletion (SMD) as function of $ASMD = SMD_{i-1} + ET_p - P \cdot R_p - I \cdot R_I$.

Once SMD is determined, ET and D are solved from Eq (4.2) and Eq (4.4) respectively.

As an alternative to logical variables, a convergent resolution method was formulated in Visual Basic for Applications (VBA) giving analogous results.

A second approach consisted in conducting the water balance differentiating per crops. Every month, the total volume of irrigation V_I (m^3) was proportionally distributed considering the percentage of occupied land and water needs per crop. The application

of WATEN resulted on discriminated series of crop evapotranspiration, ET , soil moisture depletion, SMD , and drainage, D , for each individual crop.

4.1.3.2.2 Model parameters

It was considered a sufficient number of parameters to ensure a good model performance, but low enough to avoid multiple parameters optimization solutions (Stisen *et al.*, 2008).

Model parameters are: total available moisture in the soil, TAM ; mean fraction of TAM extracted from the root zone prior to water stress, p ; ratio of irrigation use, R_I ; ratio of precipitation use, R_P and a crop evapotranspiration coefficient, C_{ET} , which is introduced as $ET_P' = ET_P \cdot C_{ET}$ where $ET_P = ET_o \cdot K_c$.

A value of $TAM = 140$ mm was initially considered following suggestions from technicians. An average value $p = 0.60$ was determined from the CROPWAT database (FAO, 2013). Two ratios of irrigation use, $R_{I1} = 0.60$, $R_{I2} = 0.80$ applied for the two detected irrigation trends (Section 4.1.4.1). For effective precipitation $P_e = P \cdot R_P$, CROPWAT (FAO, 2013) considers a fixed value $R_P = 0.80$. Initially, we considered a non-variable value of potential evapotranspiration, ET_P , with $C_{ET} = 1$.

This initial parametric vector ($TAM = 140$ mm, $p = 0.60$, $R_{I1} = 0.60$, $R_{I2} = 0.80$, $R_P = 0.80$ and $C_{ET} = 1$) was entitled *Ref0* for future considerations.

4.1.3.3 Observed and predicted data series

To assess model performance, energy consumption (E_i) was compared to analogous data derived from model results (E_{Di}). To obtain E_{Di} series, drainage volume estimated by the model (D_i), was multiplied by energy consumption per unit volume (E_{ui}), assuming an error ε_i , Eq. (4.5):

$$E_{Di} = D_i \cdot E_{ui} + \varepsilon_i \quad (4.5)$$

Where E_{ui} values were calculated as Eq. (4.6):

$$E_{ui} = \sum_{i=1}^n E_i / \sum_{i=1}^n D_i \quad (4.6)$$

To operate in terms of water volume, E_i was transformed into drainage $D_{Ei} = E_i / E_{ui}$.

The proposed model is not linear and statistical tests such as t test and F test are not applicable. The traditional correlation coefficient (ρ) was used for assessing model

performance. This coefficient is not sensible to proportional differences between observed and estimated values (Legates and McCabe, 1999). For this reason, the coefficient of efficiency (e_2) (Nash and Sutcliffe, 1970) was also implemented, Eq. (4.7):

$$e_2 = 1 - \frac{\sum (O_i - P_i)^2}{\sum (O_i - \bar{O})^2} \quad (4.7)$$

Where P_i = estimated values; O_i = observed values; $\bar{O}$ = mean observed values.

As Eq. (4.7) presents squared differences, e_2 is sensitive to outliers. To reduce this effect, the coefficient of efficiency e_l (Nash and Sutcliffe, 1970) was formulated, which is based on absolute values instead. In addition, Theil's inequality coefficient (U) (Pindyck and Rubinfeld, 1998) was implemented to measure the accuracy of data generated by the model, Eq. (4.8).

$$U = \frac{\sqrt{\sum (O_i - P_i)^2}}{\sqrt{\sum O_i^2} + \sqrt{\sum P_i^2}} \quad (4.8)$$

U is decomposed into bias (u_m), variance (u_s) and covariance (u_c) proportions, Eq. (4.9):

$$1 = u_m + u_s + u_c = \frac{(n-1) \cdot (\bar{O} - \bar{P})^2}{\sum (O_i - P_i)^2} + \frac{(n-1) \cdot (\sigma_O - \sigma_P)^2}{\sum (O_i - P_i)^2} + \frac{2(n-1) \cdot (1-\rho) \cdot \sigma_O \cdot \sigma_P}{\sum (O_i - P_i)^2} \quad (4.9)$$

A large value u_m reveals a potentially serious systematic error; when u_s dominates, the variation in the two series around their common mean differs; u_c counts for unsystematic error. Ideal Theil's proportion is $u_m \cong u_s \cong 0$, and $u_c = 1 - u_m - u_s \cong 1$.

4.1.3.4 Calibration

For model calibration, one-way sensitivity analysis was firstly performed to identify model parameters sensitivity. Secondly, a two-way sensitivity analysis identified parameters interrelations.

Model calibration was based on a robust approach based on a Monte Carlo simulations process and classical optimization:

- In the Monte Carlo process, a number of 20000 simulations were conducted. Random simulations followed uniform distributions with defined coefficients of variation. Those parametric vectors showing better model correspondence were

selected.

- An optimization of the proposed objective functions (efficiency coefficients) was performed by the Solver algorithm GRG2 (Lasdon *et al.*, 1978). As other algorithms, it gets trapped in local minima (should they exist), but permitted to corroborate and select optimal parametric vectors.

Additionally, the water balance was discriminated per crops and model calibration was conducted through a Monte Carlo simulations process. A number of 4000 simulations with parameters following normal distributions were conducted.

In a second approach, model parameters were also discriminated per crops, increasing complexity in the process and the number of parameters from 6 to 42. For model calibration, Monte Carlo was not haphazardly applied but conducted in a driven manner which permitted to diminish computational requirements, and entitled Parameters Estimation on Driven Trials (PEDT). 6000 simulations were conducted this manner. To corroborate parameters selection, the algorithm GRG2 was run for optimizing the 42-parameters vector.

4.1.4 Results and discussion

4.1.4.1 Analysis of available data series

A double-mass curve permitted to analyse data trends from 2002-2012 (Figure 4.7).

Figure 4.7 Double mass curve to analyse the data series over the study period 2002-2012, showing accumulated precipitation (P_a), irrigation (I_a), potential evapotranspiration (ET_{Pa}) and energy (E_a).

A straight line would indicate unchangeable data series. Precipitation, P , was variable over time. Irrigation, I , showed two marked trends: a first period (before month 48) with an average $I = 606$ mm/year and a second period with $I = 417$ mm/year. This 70%

irrigation reduction may be attributable to irrigation awareness, modernization or to a decrease in the salts leaching fraction (Romero-Bueno *et al.*, 2013). Potential evapotranspiration, ET_p , followed a stairs-shape behaviour due to winter and summer fluctuations. $(P+I-ET_p)$ results are closely related to drainage. A major decline occurred between months 87 and 94. This value exceeded the expected total available moisture in the soil, TAM , and might have involved a period of water deficit. Similar patterns occurred over summer periods, with an average value $P+I-ET_p = 237$ mm. $P+I$ do not fulfil crop water needs and crops might take water from the soil to avoid a reduction on evapotranspiration. Any value of TAM below 237 mm would have involved water deficit. With respect to energy, E , a downward tendency was detected over the whole studied period.

Available data series served to approach values of drainage discharge prior to the implementation of the model. The components of the water balance are shown in Table 4.2.

Table 4.2 Values of precipitation (P), irrigation (I), crop potential evapotranspiration (ET_p) and energy consumption data (E).

		P (mm)	I (mm)	ET_p (mm)	$P + I - ET_p$ (mm)	$P + I - ET_p > 0$ (mm)	E (kW·h)
Annual values	Mean	548.9	484.7	924.5	109.0	354.5	1132619
	σ (std)	180.1	148.3	41.8	150.3	138	363813
Monthly average values	1	58.73	6.45	16.77	48.40	48.7	124857
	2	69.00	7.35	28.95	47.40	49.4	133918
	3	53.49	14.52	59.05	8.97	19.1	97904
	4	52.87	51.67	88.65	15.89	22.4	109779
	5	25.20	85.74	134.51	-23.58	1.4	94356
	6	6.95	105.93	187.76	-74.89	0.0	107329
	7	3.20	104.48	167.30	-59.62	0.0	75576
	8	7.96	76.93	123.73	-38.84	0.0	53570
	9	36.18	9.34	65.21	-19.69	7.6	31087
	10	81.64	2.41	24.35	59.70	60.6	40444
	11	87.18	14.41	16.16	85.44	85.4	124129
	12	66.53	5.42	12.09	59.86	59.9	139671

Potential evapotranspiration, ET_p , was clearly exceeded by the sum up of irrigation, I , plus precipitation, P . Remarkable differences occurred from one year to another, with an average drainage value $D = 109$ mm in null water deficit conditions, $ET/ET_p = 1$. Any drainage value above $D = 109$ mm (lowest drainage boundary) would have involved crop evapotranspiration reductions.

4.1.4.2 Preliminary model results

Considering the parametric vector $Ref0$, ET values estimated by the model were 29% lower than ET_P (Table 4.3 and Figure 4.8). In summer, ET suffered dramatic reductions, close to a 50% reduction, probably due to ET_P overestimations or to an underestimation of irrigation, I .

Table 4.3 Average values of evapotranspiration (ET), soil moisture depletion (SMD) drainage (D) and energy consumption per unit volume (E_u) considering $Ref0$ ($TAM = 140$ mm, $p = 0.60$, $R_{I1} = 0.60$, $R_{I2} = 0.80$, $R_P = 0.80$, $C_{ET} = 1$).

Month	ET (mm)	ET/ET_P	SMD	D (mm)	E_u (W·h/m ³)
1	16.77	1.00	9.20	42.14	19.2
2	28.95	1.00	8.38	46.58	18.6
3	59.05	1.00	21.33	21.92	29.0
4	88.47	1.00	32.32	27.06	26.3
5	125.21	0.93	76.88	30.29	20.2
6	110.55	0.59	106.74	32.18	21.6
7	83.16	0.50	112.28	30.06	16.3
8	62.04	0.50	112.08	22.65	15.3
9	33.88	0.52	110.32	9.89	20.4
10	21.25	0.87	64.71	17.18	15.3
11	15.89	0.98	27.21	48.21	16.7
12	12.09	1.00	15.46	48.11	18.8
Year	657.3	0.71	58.1	376.3	19.5

Figure 4.8 Potential crop evapotranspiration (ET_P) and actual crop evapotranspiration (ET) considering $Ref0$ ($TAM = 140$ mm, $p = 0.60$, $R_{I1} = 0.60$, $R_{I2} = 0.80$, $R_P = 0.80$, $C_{ET} = 1$).

Accumulated drainage, D_a , was plotted against accumulated energy consumption, E_a , aiming to distinguish any trend over the years (Figure 4.9). A significant tendency

change was observed in month 78, with energy consumption per unit volume decreasing from $E_u = 22.2$ to $15.8 \text{ W}\cdot\text{h}/\text{m}^3$.

Figure 4.9 Accumulated energy consumption (E_a) versus accumulated drainage (D_a) over the study period 2002-2012 considering the model parametric vector $Ref0$. Blue dotted lines distinguish two differentiated energy consumption per unit volume trends over the study period.

This increase on energy efficiency might be a consequence of pumps replacement and/or optimized pumping management. Energy saving concerns grew after new electricity tariffs were promulgated in Spain: Royal Decree 871/2007 (MITYC, 2007).

4.1.4.3 Observed and predicted data series

4.1.4.3.1 Comparison of observed and predicted data series. Objective functions

Drainage data series derived from the model D_i were compared to drainage data derived from energy consumption D_{Ei} (Figure 4.10). Energy consumption values per unit volume $E_u = 22.2$ and $E_u = 15.8 \text{ W}\cdot\text{h}/\text{m}^3$ served to transform energy consumption data E_i into D_{Ei} data series.

Figure 4.10 Drainage series estimated by the model (D) and derived from energy data (D_E) considering $Ref0$.

Average monthly data (Figure 4.10) presented lower values of D_i over spring and greater values of D_i over summer compared to drainage data series D_{Ei} . This might be a consequence of estimating irrigation data from water allocated to Melendo reservoir instead of counting with flowmeter irrigation data (Section 4.1.3.1, Figure 4.2). Water takes time to reach drainage pumping stations and individual monthly drainage D_{Ei} (Figure 4.10) was expected to present a certain delay in comparison with D_i . However, this effect might have been compensated with the effect of estimating the irrigation based on Melendo reservoir data.

The correlation coefficient value attained $\rho = 0.96$, 0.90 and 0.87 ; the coefficient of efficiency reached $e_2 = 0.93$, 0.80 and 0.74 , and Theil's inequality coefficient resulted $U = 4.3\%$, 8% , and 18% for average annual, average monthly and monthly individual values respectively. In every case, Eq. (4.9) fitted the ideal Theil's proportion distribution, resulting in a good model performance.

A multiple linear regression comprising P , I and ET_o data series would result in D_i - D_{Ei} correlation coefficients $\rho = 0.93$, $\rho = 0.74$ and $\rho = 0.5$, for average annual, monthly and monthly individual series, much lower values compared to model results.

4.1.4.4 Calibration

4.1.4.4.1 One-way sensitivity analysis

To determine the sensitivity of the model to parameters variation, one-way sensitivity analysis was performed (Figure 4.11).

Figure 4.11 Sensitivity analysis of model parameters: total available moisture in the soil (TAM), readily available fraction of TAM ($p=RAM/TAM$), effective precipitation fraction (R_p), irrigation efficiency (R_i) and crop evapotranspiration coefficient (C_{ET}).

The variation of total available moisture in the soil, TAM , mainly affected autumn and winter results. Higher values of TAM produced lower values of D and higher values of ET/ET_p ratio and E_u . Best correlation, ρ , and efficiency, e_2 , coefficients were achieved with $TAM = 125$ and $TAM = 160$ mm for annual and monthly average values respectively.

Model sensitivity to parameter p (TAM fraction taken from the root zone prior to water stress), was significant over autumn and winter periods. An increase over p in a range from 0.1 up to 1 produced lower volumes of D and a greater ET/ET_P ratio. Maximum model performance was close to $p = 0.7$.

Considering the two detected irrigation trends (Section 4.1.4.1), two parameters were distinguished for analysing model sensitivity to irrigation efficiency: R_{I2} in a range from 0.5 up to 1; R_{I1} fixed as $R_{I1} = 6/8 \cdot R_{I2}$. Higher values of R_I produced lower values of D over spring and summer (decreasing from 495 to 300 mm), and lower ET/ET_P ratios and E_u values. Best model performance came up with $R_{I2} = 0.85$.

Model sensitivity to precipitation efficiency, R_P , in a range from 0.6 up to 1 produced smaller values of D over summer. Higher R_P values in autumn increased soil moisture content. As a consequence, winter rainfall resulted in runoff, producing higher values of drainage, D , over the months of November and December. Higher R_P values produced greater ET/ET_P ratios and E_u values. Model performance improved when $0.75 \leq R_P \leq 0.85$.

Model sensitivity to the crop evapotranspiration coefficient, C_{ET} , in a range from 0.75 to 1.25 led to lower D values and a reduced ET/ET_P ratio. Summer months were not sensible to C_{ET} due to water deficit conditions. Best correlation values corresponded to $0.8 \leq C_{ET} \leq 0.85$.

The sensitivity analysis demonstrated a notable effect of R_I over summer months. Parameters TAM and p had a marked effect over winter, pointing to a significant correlation between them.

4.1.4.4.2 Two-way sensitivity analysis

TAM and p values were simultaneously modified while fixing the remaining model parameters. As shown in Figure 4.12, the maximum value of e_2 , close to 0.825, results from different combinations of p and TAM parameters.

Figure 4.12 Coefficient of efficiency (e_2) and drainage (D) with different TAM - p combinations, considering $Ref0$ ($R_{I1} = 0.60$, $R_{I2} = 0.80$, $R_P = 0.80$, $C_{ET} = 1$).

Drainage, D , gradually declined when TAM and p values simultaneously increased. Isoquants e_2 and D are almost coincident.

4.1.4.4.3 Monte Carlo Simulations Process

A number of 20000 simulations were conducted through random parameters variation following uniform distributions. The range of parameters variations were: TAM (50-300 mm), p (0-1), R_{I1} (0.4-1), R_{I2} (0.5-1), R_P (0.6-1) and C_{ET} (0.75-1.25). Best 40 out of 20000 simulations attaining higher model performance were selected. Optimization of either e_2 or e_1 criteria did not encounter significant differences. Table 4.4 shows model calibration in terms of e_2 criteria, and correlation matrix amongst parameters is shown in Table 4.5.

Table 4.4 Results of the 40 simulations (out of 20000) with highest coefficient of efficiency e_2 following a Monte Carlo.

e_2	TAM	p	R_{I1}	R_{I2}	R_P	C_{ET}	D	ET	E_{u1}	E_{u2}	ρ	e_2	e_1	U
mean	208.6	0.59	0.70	0.80	0.86	0.87	341.7	693.5	25.4	16.9	0.93	0.866	0.65	0.094
stdev	44.1	0.21	0.05	0.04	0.04	0.07	28.4	28.1	2.67	1.14	0.00	0.01	0.01	0.005

Model parameters: TAM , p , R_{I1} , R_{I2} , R_P , C_{ET}

Model results: drainage (D), crop evapotranspiration (ET), energy consumption per unit volume (E_{u1} and E_{u2})

Objective functions: correlation coefficient (ρ), coefficients of efficiency, (e_2 and e_1), Theil's inequality coefficient (U)

Table 4.5 Correlation matrix considering the 40 simulations (out of 20000) with highest coefficient of efficiency e_2 following a Monte Carlo.

ρ	TAM	p	R_{II}	R_{I2}	R_P	C_{ET}
TAM	1.00	-0.90	0.22	0.11	0.14	0.15
p		1.00	-0.23	-0.16	0.07	-0.22
R_{II}			1.00	-0.29	0.01	0.66
R_{I2}				1.00	-0.28	0.11
R_P					1.00	0.13
C_{ET}						1.00

Mean values of TAM resulted higher than expected; mean p values were close to initial values taken from CROPWAT (FAO, 2013); an increase on the previously considered values of R_P and R_{II} and a reduction on C_{ET} improved model performance.

The resulting value of drainage $D = 342$ mm was slightly lower than $D = 376$ mm which resulted when considering the initial parametric vector $Ref0$ (Table 4.3).

Drainage resulted notably dependent on the assigned TAM and p values, and these results may be cautiously considered.

4.1.4.4.4 Optimization GRG2

Excel Solver algorithm, GRG2, was implemented to corroborate selected parametric vectors. Model performance improved in comparison with the implementation of the initial parametric vector $Ref0$ (Table 4.6).

Table 4.6 Model results for different parametric vectors.

Criteria	TAM	p	R_{II}	R_{I2}	R_P	C_{ET}	e_2	e_1	D	ET/ET_p	Vector
$Ref0, K_c CROPWAT$	140	0.60	0.60	0.80	0.80	1.00	0.82	0.62	376	0.71	1
Optimization e_2	145	1.00	0.68	0.78	0.85	0.80	0.89	0.68	365	0.96	2a
e_1	138	1.00	0.69	0.79	0.85	0.75	0.88	0.68	383	0.95	2b
e_2	193	0.67	0.71	0.79	0.84	0.85	0.89	0.68	341	0.89	3
$e_2, p = 0.6$	204	0.60	0.70	0.79	0.85	0.84	0.89	0.67	345	0.89	4
$e_2, p = 0.6, C_{ET} = 1$	196	0.60	0.78	0.79	0.86	1.00	0.87	0.66	302	0.79	5
$Ref1, K_c CROPWAT$	170	0.60	0.70	0.80	0.85	0.88	0.87	0.66	353	0.84	6a
$Ref1, K_c = K_{cb CHG}$	170	0.60	0.70	0.80	0.85	1	0.87	0.67	357	0.83	6b

Both coefficients of efficiency e_1 and e_2 improved when optimizing the model by the algorithm GRG2 (Table 4.6). On average, the value of e_1 increased from 0.62 up to 0.68, and the value of e_2 improved from 0.82 up to 0.89, vector 2. We obtained different parametric vectors dependent on the starting point, vector 2 and 3. Vector 2, presenting lower values of TAM and greater values of p , produced higher values of D and greater ET/ET_p ratios in comparison with vector 3.

Compared to *Ref0*, model performance improved when increasing values of TAM , p , R_{II} and R_P values. In terms of C_{ET} , model performance improved when reducing the initial estimated potential evapotranspiration ET_P . As a consequence, and maintaining $p = 0.60$ (vector 4, 5 and 6), a new parametric vector *Ref1* was implemented ($TAM = 170$ mm, $p = 0.6$, $R_{II} = 0.70$, $R_P = 0.85$), vector 6. Considering *Ref1*, model results presented a 12% ET_P reduction, vector 6a. For making effective this reduction on ET_P , basal crop coefficients, K_{cb} , were considered. the model was run with *Ref1* and K_{cb} values as crop coefficients, vector 6b. The value of drainage, D , decreased from 376 to 357 mm/year whereas energy consumption per unit volume, E_u , increased from 19.5 to 20.6 W·h/m³. In terms of actual crop evapotranspiration, ET , it went up from 657 to 676 mm/year (Table 4.7).

Table 4.7 Average values of evapotranspiration (ET), soil moisture depletion (SMD) drainage (D) and energy consumption per unit volume (E_u), considering *Ref1* ($TAM = 170$ mm, $p = 0.60$, $R_{II} = 0.70$, $R_{I2} = 0.80$, $R_P = 0.85$, $C_{ET} = 1$).

Month	ET (mm)	ET/ET_P	SMD	D (mm)	E_u (W·h/m ³)
1	13.68	1.00	8.64	43.77	18.5
2	25.42	1.00	6.29	48.58	17.9
3	52.59	1.00	15.03	24.17	26.3
4	69.97	1.00	10.66	30.20	23.6
5	107.80	1.00	32.50	24.98	24.5
6	153.90	0.92	100.56	27.03	25.8
7	105.71	0.67	124.22	25.64	19.1
8	70.69	0.60	129.43	19.42	17.9
9	33.82	0.61	125.41	7.69	26.2
10	21.71	0.89	75.98	12.91	20.3
11	12.03	0.99	32.18	45.76	17.6
12	9.08	1.00	16.36	47.05	19.3
Year	676.4	0.83	56.4	357.2	20.6

Ref1 model results were analogous to those after considering *Ref0* (Figure 4.10) and have not been plotted.

4.1.4.5 Model results discriminating per crops

For each crop, a water balance was performed. Considering *Ref1* ($TAM = 170$ mm, $p = 0.60$, $R_{II} = 0.70$, $R_{I2} = 0.80$, $R_P = 0.85$, $C_{ET} = 1$ and basal crop coefficient values K_{cb}), model results showed slightly lower ET values and a higher value of D (Table 4.8) in comparison with no discrimination per crops (Table 4.7).

Table 4.8 Average values of evapotranspiration (ET), soil moisture depletion (SMD) drainage (D) and energy consumption per unit volume (E_u) considering $RefI$ and a water balance for each crop.

Month	ET (mm)	ET/ET_p	SMD	D (mm)	E_u
1	13.6	0.99	10.2	43.7	18.5
2	25.4	1.00	10.7	51.4	16.9
3	52.4	1.00	24.0	28.3	22.5
4	69.1	0.99	25.4	37.5	19.0
5	105.0	0.97	47.6	28.1	21.8
6	136.3	0.82	98.1	27.0	25.8
7	110.4	0.70	126.4	25.6	19.1
8	74.0	0.63	134.9	19.4	17.9
9	32.0	0.57	129.1	7.7	26.2
10	21.1	0.87	79.6	13.7	19.2
11	11.7	0.96	34.2	44.6	18.1
12	9.1	1.00	18.1	46.8	19.4
Year	660	0.81	61.5	374	19.7

Model performance improved, particularly in terms of average monthly data (Figure 4.13). The average coefficient of efficiency e_2 increased from 0.87 to 0.90; e_1 improved from 0.67 to 0.74.

Figure 4.13 Results of drainage series estimated by the model (D) and derived from energy (D_E) considering $RefI$ and water balance discriminated per crops.

Model calibration was performed through a Monte Carlo simulations process. A number of 4000 simulations were conducted through random parameters variation. Simulations followed normal distributions, with average values equal to the parametric vector *RefI* and a variation coefficient $CV = 0.10$. The variation of the outputs was lower in comparison, Table 4.9.

Table 4.9 Model results after 4000 simulations nearby *RefI* with $CV = 0.1$.

	<i>ET</i>	<i>D</i>	<i>E_{u1}</i>	<i>E_{u2}</i>	<i>e₂</i>	<i>e₁</i>
Reference 1	660	374	22.5	15.7	0.90	0.74
Mean	375	659	22.5	15.8	0.86	0.60
<i>CV</i>	0.066	0.038	0.059	0.083	0.059	0.076

Ordering the resulting 4000 parametric vectors from higher to lower values of either e_2 or e_1 criteria, the parametric vector *RefI* corresponded to the 72nd and 63rd place respectively. Although *RefI* solution is not the optimal, it approached a local minimum. As a consequence, the haphazard calculation of model parameters may worsen model performance. Table 10 sums up some statistics of the 40 out of 4000 simulations with highest values of e_2 .

Table 4.10 Model parameters and statistics considering the 40 out of 4000 simulations (nearby *RefI* for a water balance per crops; $CV = 0.1$) with higher value e_2 .

	<i>TAM</i>	<i>p</i>	<i>R_{I1}</i>	<i>R_{I2}</i>	<i>R_P</i>	<i>D</i>	<i>ET</i>	<i>E_{u1}</i>	<i>E_{u2}</i>	<i>e₂</i>	<i>e₁</i>
Average	182.3	0.624	0.695	0.803	0.871	362.1	671.7	23.2	16.3	0.901	0.74
<i>CV</i>	0.038	0.068	0.034	0.019	0.016	0.017	0.009	0.022	0.018	0.001	0.006

4.1.4.5.1 Model results per crops considering model parameters discrimination

Aiming to differentiate model parameters amongst crops, the number increased from 6 parameters to 42 (6 x 7 crops). *TAM* depends on root depth, but in shallow soil depth conditions, it might not be applicable. In the case of *p*, CROPWAT (FAO, 2013) assigns different values amongst crops. Irrigation efficiency, *RI*, mainly depends on the irrigation system and considered crop.

For model calibration, Excel Solver was run for optimizing the 42-parametric vector. Model performance improved, $e_2 = 0.93$. Due to the elevated number of model parameters, a Monte Carlo simulations process would require an exponential number of simulations to attain a parametric vector nearby the optimum (should it exist). In order to reduce the number of simulations, Monte Carlo was not haphazardly applied but driven in a manner which permitted to diminish computational requirements. On a similar manner to genetic algorithms, variations on parameters were driven in the

direction of better model performance. To this end, consecutive sets of 200 simulations were conducted, until a number of 6000 simulations were reached. The best model performance vector was selected, and the next 200 simulations were performed around this value as the mean of a normal distribution with $CV = 0.1$. Model performance was analogous to the obtained through Solver but with the advantage of obtaining a wide range of parameters values with good model performance. Nevertheless, this solution relied on parameters discrimination per crops in a non-always justifiable manner.

4.1.5 Conclusions

We assessed the water balance and calculated the flow rate discharged from an irrigation district with scarce available data to a receiving water body. Energy consumption for drainage discharge was used for model calibration. The proposed hydrological model WATEN attained an average Nash-Sutcliffe coefficient $e_2 \cong 0.90$ between observed and estimated drainage discharge.

A double-mass curve permitted to detect data trends on irrigation and energy consumption throughout the years, leading to crucial improvements on its performance (from $e_2 \cong 0.72$ to 0.90).

Available data did not permit to distinguish between total available moisture and readily available moisture in the soil, attaining wide-ranging *TAM-RAM* combinations that maximise model performance.

Calibration through Solver encountered higher values of e_2 compared to robust model calibration through Monte Carlo. However, Solver solutions were occasionally dependent on the starting point. In contrast, Monte Carlo enabled to visualize a broad space of surrounding best model parametric vectors.

A water balance per crops, with the same parametric vector, improved model performance (from $e_2 = 0.87$ to 0.90). A parametric vector for each crop increased e_2 from 0.90 to 0.93, although it resulted on non-always justifiable parameters.

Model calibration based on a Monte Carlo approach and driven on a simplified manner of genetic algorithms (Parameters Estimation on Driven Trials, PEDT) resulted necessary to diminish computational requirements in the case of model parameters discrimination per crops.

A significant 29% and 17% crop evapotranspiration reduction was detected by implementing either widely spread or regionalized crop evapotranspiration coefficients. Average water discharge was close to 3740 m³/ha/year, probably sufficient for leaching irrigation water salts.

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4.2 Study II. Vegetation water use based on a thermal and optical remote sensing model in the Mediterranean region of Doñana

Abstract: Terrestrial evapotranspiration (*ET*) is a central process in the climate system, the major component in the terrestrial water budget, and responsible for the distribution of water and energy on land surfaces, especially in arid and semiarid areas. In order to inform water management decisions particularly in water scarcity environments, it is important to assess *ET* vegetation use by differentiating irrigated socio-economic areas and natural ecosystems. The global remote sensing *ET* product MOD16 has proven to underestimate *ET* in semiarid regions, where *ET* is very sensitive to soil moisture. The objective of this research was to test whether the thermally-modified remote sensing *ET* model (PT-JPL-thermal), proven to perform well in drylands at Eddy Covariance flux sites using the land surface temperature as a proxy to the surface moisture status, could be up-scaled at regional levels and introducing modelled net radiation. We applied three methods to track the spatial and temporal characteristics of *ET* in the World Heritage UNESCO Doñana region: i) a locally calibrated hydrological model (WATEN); ii) the PT-JPL-thermal; and iii) the global remote sensing *ET* product MOD16. The PT-JPL-thermal showed strong agreement with the WATEN *ET* in-situ calibrated estimates ($\rho=0.78$; $\rho_{1\text{month-lag}} = 0.94$), though the MOD16 product did not ($\rho=0.48$). The thermally modified PT-JPL approach has proven to be a strong remote sensing model for detecting *ET* at regional level in semiarid environments, requiring only air temperature and incoming solar radiation from climatic databases apart from standard satellites-products freely available.

4.2.1 Introduction

The global water cycle is changing due to the combined effects of climate change and human interventions over the 21st century (Prudhomme *et al.*, 2014). One of the greatest challenges is keeping water consumption at sustainable levels, more complex due to increasing population in a context of climate uncertainty (Alexandratos and Bruinsma, 2012; Schewe *et al.*, 2014) and 3.5-4.4 billion people estimated under water scarcity conditions in 2050 (Flörke *et al.*, 2018). Many regions of the world can expect a combination of increasing temperatures (largely increasing evaporative demand) and decreasing precipitation patterns, leading to increased stress on tackling water demand (Curtis *et al.*, 2014). A prime example of this is the Mediterranean region, consistently

projected as a “hotspot” of drying trends and prolonged water scarcity conditions (Hoerling *et al.*, 2012; Tanasijevic *et al.*, 2014).

The Iberian Peninsula is predicted to be amongst the most affected areas by severe droughts by the end of the 21st century (Diffenbaugh *et al.*, 2007). In this region, where irrigated agriculture represents over 80% of the total extracted water (Minacapilli *et al.*, 2016), land use shifts towards higher market-valued crops represent a major driver of change which will markedly increase water withdrawals (Lambin *et al.*, 2001). In the Guadalquivir basin in Spain, irrigation water requirements are expected to increase between 15 and 20 per cent by 2050 (Chavez-Jimenez *et al.*, 2015). This may cause a redistribution of water between surface and groundwater (Scanlon *et al.*, 2007); monitoring more closely the variations in the hydrological cycle components, among them evapotranspiration *ET*, is of major importance in countries facing intensified drought spills (Oki and Kanae, 2006; Chirouze *et al.*, 2014).

After precipitation, *ET* is the major component in the terrestrial water budget (Leuning *et al.*, 2008). Evapotranspiration at specific locations can be estimated by using methods such as lysimeters, Bowen-ratio or Eddy Covariance (EC) amongst others (Allen *et al.*, 2011). However, *ET* estimations at large-scales are complex to achieve due to spatial heterogeneity in the land surface (Anderson *et al.*, 2003; Wang *et al.*, 2010; Song *et al.*, 2017). As the only connecting term between the water cycle and the land surface energy budget (Guzinski *et al.*, 2015; Xing *et al.*, 2016), *ET* can be estimated by hydrological models (HMs) relying on the water balance, or by land surface models (LSMs) computed through the mass-transfer equations between the land surface and the atmosphere (Senay *et al.*, 2011).

Conceptual HMs consider an undivided entity with individual values of input variables and parameters (Beven and Freer, 2001); on the other hand spatially distributed HMs or prognostic LSMs enable *ET* to be estimated at large scales in a spatially explicit manner (Fortin *et al.*, 2006). This type of models requires a priori information on land use and surface properties, which are not always up-to-date, and may be complex to retrieve in situations of fast land use changes, for instance new irrigation developments. Diagnostic RS-LSM models need limited a priori data on soil and vegetation parameters to estimate *ET*, and can rely on RS-land surface temperature (*LST*) as a proxy to the surface moisture status (Yilmaz *et al.*, 2014).

The complexity of RS-based models to retrieve ET depends on the process equations considered (Kalma *et al.*, 2008; Karimi and Bastiaanssen, 2015). ET can be directly estimated as a residual of the surface energy equation or based on potential evapotranspiration adjusted to actual rates using different constraints factors from remote sensing. The Penman-Monteith (PM) equation (Monteith, 1965; Allen *et al.*, 1998) is the base to compute ET in some global RS- ET products such as the first widely available ET product MOD16 (Mu *et al.*, 2007a; Mu *et al.*, 2011), whose main challenge relies on the estimation of surface and aerodynamic resistances to the water vapor (Zhang *et al.*, 2010). Hu *et al.* (2015) found that MOD16 best performs in temperate and fully humid climates and produces a consistent underestimation of ET in semiarid regions such as Spain, Portugal, the neighborhood of the Black Sea and the Caspian Sea (Hu *et al.*, 2015), and semiarid climatic zones in the conterminous United States (Velpuri *et al.*, 2013). In these regions and under water stress conditions, ET is very sensitive to soil moisture. In MOD16, canopy resistance to water vapor uses vegetation-related RS inputs (e.g. LAI) and stomatal conductance, whereas soil resistance to water vapor relies on the vapor pressure deficit (VPD) and relative humidity (RH) as indicators of water stress (Mu *et al.*, 2007a; Mu *et al.*, 2011). The Priestley-Taylor equation (Priestley and Taylor, 1972) bridges the limitation of estimating these resistances by using an empirical multiplier α_{PT} (Zhang *et al.*, 2009). The Priestley-Taylor Jet Propulsion Laboratory (PT-JPL) combines the PT-approach with the reduction of potential ET based on ecophysiological constraints to land-atmosphere water fluxes (Fisher *et al.*, 2008). With the aim to minimize the need for RH climatic reanalysis data, and to improve the performance in semiarid regions, García *et al.* (2013) proposed a modification of the PT-JPL model (PT-JPL-thermal herein) by introducing the LST with a thermal inertia approach as a proxy to the soil moisture status.

This approach has proven to perform well in drylands, under Mediterranean and monsoonal conditions, and to perform better than other RS models as the PM model adapted by Leuning *et al.* (2008). Although the PT-JPL-thermal model has been benchmarked at EC flux sites (García *et al.*, 2013), it has not been yet tested with modelled net radiation or at regional levels.

The main objectives of this work were: (i) to assess whether the RS PT-JPL-thermal model that uses the thermal inertia approach for soil evaporation, can perform similarly

to a hydrological model calibrated with in-situ data that requires soil moisture-associated parameters to retrieve *ET*; (ii) to compare and assess the *ET* derived from the PT-JPL-thermal against the global *ET* product MOD16, which estimates soil evaporation as a function of *VPD* and *RH* climatic reanalysis, in the Mediterranean region of Doñana including natural ecosystems (wetland, shrubland, coniferous forest) and irrigated areas (mixed-irrigated areas and rice fields).

4.2.2 Study area

The study area presents Mediterranean climate and Atlantic influence, warm and dry summers and temperate and semi-humid winters; temperatures range from 24°C average in summer to 10°C average in winter (Muñoz-Reinoso, 2018), average rainfall is about 560 mm, more than 80% occurring between October and March. The study area covers the Doñana National Park (54251 ha) differentiating three natural ecosystems: seasonal wetlands, shrublands and coniferous forests, which rest over the aquifer Almonte-Marismas, extensive rice fields (García De Jalón *et al.*, 2014) on the right and left bank of the Guadalquivir river, and mixed-irrigation croplands established in ancient marshes. In particular, the mixed-irrigation BXII, converted into arable land since 1960s (Martín-López *et al.*, 2011) is one of the most-water-intensive irrigated areas in the Guadalquivir basin, with approximately 15000 hectares and above 6000 m³/ha per year.

The study area is of great international importance; the Doñana National Park is included in the Ramsar Convention as one of the largest wetlands in Europe (Green *et al.*, 2017b), designated a World Heritage Site by UNESCO in 1995, and buffered by a Natural Park, which entered the endangered Montreux Record of Ramsar sites in 1990 (Serrano *et al.*, 2016). The high variability of land uses in the Doñana region, where conflicts between the environment conservation and socio-economic development have increased (García-Novo and Marín-Cabrera, 2006) makes this region a particularly interesting water-scarcity hot-spot for the assessment of water demand on different land uses and water availability conditions.

4.2.3 Materials and methods

4.2.3.1 Remote sensing dataset

Multiple remote sensing observations were acquired from the Moderate Resolution Imaging Spectroradiometer (MODIS), using sensors from both Aqua and Terra satellites. Satellite data were used in combination with *in situ* meteorological data (air

temperature and radiation) as inputs for the PT-JPL-thermal model. MODIS land products were retrieved from The Earth Observing System Data and Information System (EOSDIS), a core capability in National Aeronautics Space Administration (NASA) Earth Science Data Systems Program. All the selected MODIS products (version 5) were acquired at 1km pixel resolution for the study period 2003-2012. The temporal resolution of the data sets were: (1) daily for Land Surface Temperature (LST) and Emissivity ($Emis$) from MOD11A2 and MYD11A2; (2) 8-day-composites of Leaf Area Index (LAI) and Fraction of Photosynthetically Active Radiation (f_{APAR}) from MOD15A2, broadband surface albedo (α) acquired from MCD43B3 and (3) 16-day-composites of Normalized Difference Vegetation Index ($NDVI$) retrieved from MOD13A2. For the 8 and 16 day-composites variables, the same value was used for the entire period.

4.2.3.2 Meteorological data

Meteorological data were obtained from the agro-climatic station Lebrija I (36.98°N, 6.13°W, <https://www.juntadeandalucia.es/agriculturaypesca/ifapa/ria/>), a station site of the Agroclimatic Information Network of Andalusia (RIAA). This station is controlled by a CR10X datalogger (Campbell Scientific) with sensors to measure T_{air} (T_{max} , T_{min} and T_{mean}), relative humidity RH (RH_{max} , RH_{min} , RH_{mean}), solar radiation R_s , precipitation P , wind speed and direction, and reference evapotranspiration ET_o , transferred by GSM modems for quality control and data validation (Estévez *et al.*, 2011).

4.2.3.3 Remote sensing ET model (PT-JPL-thermal)

The PT-JPL-thermal model is described in (García *et al.*, 2013), a thermally modified version of the PT-JPL model of Fisher *et al.* (2008). In this work, the PT-JPL-thermal model was spatially distributed over the study area for a 10 years-period at a daily time-scale. Daily estimations provided by the model were further aggregated per month to be comparable to the other evaluated models' temporal-scale. The PT-JPL-thermal model retrieves actual evapotranspiration (ET), in mm/day by estimating actual canopy transpiration (ET_c) and soil evaporation (ET_s) as two layers (Eq. 4.10). The quantity of water intercepted by the canopy was not considered in the formulation of the model as in García *et al.* (2013).

$$ET = ET_c + ET_s \quad (4.10)$$

To simplify the comprehension of the model, all the equations and variables used to retrieve the ET as the combination of canopy transpiration and soil evaporation are detailed in Table 1.

Canopy transpiration

Potential canopy evapotranspiration ETp_c was downscaled to actual ET_c by determining the fraction of the canopy actively transpiring (f_g) and reductions on potential transpiration due to a moisture constraint (f_m) and a temperature constraint (f_t) for canopy transpiration.

The green canopy fraction (f_g) is the ratio between absorbed (f_{APAR}), acquired from the 8-day-composite MOD15A2, and intercepted (f_{IPAR}) photosynthetic active radiation by the vegetation cover, estimated as a function of the Normalized Difference Vegetation Index ($NDVI$) acquired from the 16-day-composite MOD13A2 as in Fisher *et al.* (2008). The plant moisture constraint (f_m) considers a reduction of light utilization for canopy transpiration in response to water stress (Fisher *et al.*, 2008). The plant temperature constraint (f_t) considers a decrease on canopy transpiration when the temperature differs from an optimum temperature range and was computed by following the Carnegie-Ames-Stanford Approach model (CASA) (Potter *et al.*, 1993; García *et al.*, 2013).

Soil evaporation

Potential soil evaporation ETp_s was downscaled to actual ET_s by applying a soil moisture constraint (f_{sm}) as in García *et al.* (2013). The soil thermal inertia (TI), can be indicative of soil moisture content variations (Peters *et al.*, 2011). A simple approximation to this concept is the apparent thermal inertia (ATI) derived from multi-spectral remote sensing images (Mitra and Majumdar, 2004; Verstraeten *et al.*, 2006). ATI results from combining the RS surface albedo α , maximum daily land surface temperature oscillations ($LST_{Day} - LST_{Night}$) and a solar flux correction factor C (Table 4.11). The formulation of f_{sm} based on ATI in this paper relies on the minimum and maximum seasonal ATI , respectively. Assuming that maximum ATI values occur at saturated soil moisture content conditions and that minimum ATI corresponds to the residual soil moisture content in the soil, f_{sm} would approximate the difference between actual soil moisture content and field capacity (Verstraeten *et al.*, 2006).

Table 4.11 Equations and variables used to estimate daily values of ET in the PT-JPL-thermal model. $\alpha_{PT}=1.26$, Pt coefficient; Δ , slope of the saturation-to-vapor pressure curve (Pa K^{-1}); γ , psychrometric constant ($0.066 \text{ kPa } ^\circ\text{C}^{-1}$); G , soil heat flux (Wm^{-2}) minimal at the monthly scale as in Fisher et al. (2008); σ , Stefan-Boltzmann constant ($5.67 \times 10^{-8} \text{ Wm}^{-2}$); c and d , constants (0.261 and 7.77×10^{-4} respectively); T_{max} and T_{min} ($^\circ\text{C}$), min and max climatic T_{air} (IFAPA, 2014); N (h), time lag between sunrise and sunset (<https://www.esrl.noaa.gov/gmd/grad/researchp.html>); d , time lag for maximum temperature before sunset (1.86 h); $MODIS_{time}$ from MYD11A2; c , time lag for minimum air temperature after sunrise (-0.17 h); ε_s , average of emissivity bands 31 and 32; LST from MYD11A2; $R_{s_{day}}^{\downarrow}$ ($\text{MJ/m}^2/\text{day}$), climatic (IFAPA, 2014); α_{BSA} and α_{WSA} , broadband black and white-sky albedo; t (h), time lag between sunrise time from NOAA and $MODIS_{time}$; f_{APAR} , fraction of absorbed photosynthetically active radiation; f_{IPAR} , fraction of intercepted photosynthetically active radiation; T_{opt} , optimum temperature for plant growth (25°C); T_{amp} , daily mean T_{air} ($^\circ\text{C}$); $(LST_{Day} - LST_{Night})$, maximum daily LST oscillations; ϑ , latitude; φ , solar declination factor.

Variable description	PT-JPL-thermal equations	Reference
Evapotranspiration	$ET = ET_c + ET_s$	Fisher et al. (2008)
Canopy transpiration	$ET_c = ET_{pc} \cdot f_g \cdot f_m \cdot f_t$	Fisher et al. (2008)
Potential canopy transpiration	$ET_{pc} = \alpha_{PT} \cdot \frac{\Delta}{\Delta + \gamma} \cdot (R_{nc} - G)$	Fisher et al. (2008)
• Net canopy radiation	$R_{nc} = R_n - R_{ns}$	Fisher et al. (2008)
• Net soil radiation	$R_{ns} = R_n \cdot e^{(-k_{Rn} \cdot LAI)}$	Norman et al. (1995)
• Net radiation	$R_n = R_L^{\downarrow} - R_L^{\uparrow} + R_S^{\downarrow} - R_S^{\uparrow} = R_L + R_S$	Fisher et al. (2008)
<u>Instant. incoming longwave radiation</u>	$R_{L_{inst}}^{\downarrow} = \sigma \cdot (T_{airMODIS-time} + 273.15)^4 \cdot \left[1 - \left(c \cdot e^{(-d \cdot (T_{airMODIS-time})^2)} \right) \right]$	Idso and Jackson (1969)
<u>Air temperature at MODIS pass-time</u>	$T_{airMODIS-time} = (T_{max} - T_{min}) \cdot \sin\left(\frac{\pi \cdot m}{N+2 \cdot d}\right) + T_{min}$	Parton and Logan (1981)
<u>Nb.of hours from T_{min} until sunset</u>	$m = MODIS_{time} - \left(12 - \left(\frac{N}{2} \right) + c \right)$	Parton and Logan (1981)
<u>Instant. outgoing longwave radiation</u>	$R_{L_{inst}}^{\uparrow} = -\varepsilon_s \cdot \sigma \cdot LST^4$	García et al. (2007)
<u>Daily shortwave radiation</u>	$R_{S_{day}} = R_{S_{day}}^{\downarrow} \cdot (1 - \alpha)$	García et al. (2007)
<u>Albedo</u>	$\alpha = 0.8 \cdot \alpha_{BSA} + 0.2 \cdot \alpha_{WSA}$	Rasmussen et al. (2014)
<u>Instant. shortwave radiation</u>	$R_{S_{inst}} = \frac{R_{S_{day}}}{J} \cdot \frac{24}{N}$	Jackson et al. (1983)
<u>Conversion factor day-inst</u>	$J = \frac{2}{\sin\left(\frac{\pi \cdot t}{N}\right)}$	Jackson et al. (1983)
<u>Instantaneous net radiation</u>	$R_{n_{inst}} = R_{L_{inst}}^{\downarrow} + R_{S_{inst}}$	
<u>Daily net radiation</u>	$R_{n_{day}} = R_{n_{inst}} \cdot J \cdot \frac{N}{24}$	Bisht et al. (2005)
Canopy transpiration constraints		
• Green canopy fraction	$f_g = f_{APAR}/f_{IPAR}$	Fisher et al. (2008)
• Plant moisture constraint	$f_m = \frac{f_{APAR}}{f_{APARmax}}$	Fisher et al. (2008)
• Plant temperature constraint	$f_t = 1.1814 / \left[\left(1 + e^{0.2 \cdot (T_{opt} - 10 - T_{am})} \right) \right] / \left[\left(1 + e^{0.3 \cdot (-T_{opt} - 10 + T_{am})} \right) \right]$	García et al. (2007)
Soil evaporation	$ET_s = ET_{ps} \cdot f_{sm}$	Fisher et al. (2008)
Potential soil evaporation	$ET_{ps} = \alpha_{PT} \cdot \frac{\Delta}{\Delta + \gamma} \cdot (R_{ns} - G)$	Fisher et al. (2008)
Soil evaporation constraints		
• Soil moisture constraint	$f_{sm} = \frac{ATI - ATI_{min}}{ATI_{max} - ATI_{min}}$	García et al. (2013)
<u>Apparent thermal inertia</u>	$ATI = C \cdot \frac{1 - \alpha}{(LST_{Day} - LST_{Night})}$	García et al. (2013)
<u>Solar flux correction factor</u>	$C = \sin\vartheta \cdot \sin\varphi \cdot (1 - \tan^2\vartheta \cdot \tan^2\varphi) + \cos\vartheta \cdot \cos\varphi \cdot \arccos(-\tan\vartheta \cdot \tan\varphi)$	Iqbal (1983)

4.2.3.4 Hydrological model WATEN

WATEN is a conceptual model that approaches water balances where streamflow data are not available. Developed in Moyano *et al.* (2015), it was applied to the mixed-irrigation BXII District, where the model was calibrated with energy data to pump the drainage discharge. WATEN requires climatic, crop-soil and farm management data, and relies on the water balance (Eq. 4.11) to solve ET and drainage (D) based on changes in soil moisture (S), in mm/month.

Considering $\Delta t = 1$ month, we get:

$$P_i + I_i = ET_i + D_i + S_i - S_{i-1} \quad (4.11)$$

Where P_i is precipitation in month i , I_i is irrigation, D_i is drainage, and $(S_i - S_{i-1})$ is soil moisture variation between one month and the preceding.

To estimate ET , potential crop evapotranspiration ET_p is adjusted from reference evapotranspiration ET_o by local basal crop coefficient values and downscaled according to soil moisture variations. The maximum amount of water retained by the soil and made available to the plant, is characterized by the total available moisture (TAM). When moisture depletion reaches this value, the plant would not extract any water and transpiration would not occur. The readily available moisture (RAM) is a fraction of TAM depending on the crop and its development phase. Soil moisture depletion ($SMD \equiv TAM - S$), the amount of water depleted from the root zone, facilitates the estimation of losses and gains estimates of the water budget (Allen *et al.*, 1998), expressed as $S_i - S_{i-1} = -(SMD_i - SMD_{i-1})$. When the depletion level is below RAM , ET reaches potential levels; for a moisture depletion between RAM and TAM levels, ET is reduced from potential levels (Eq. 4.12).

$$ET = \begin{cases} ET_p, & SMD \leq RAM \\ ET_p \cdot \frac{TAM - SMD}{TAM - RAM}, & SMD > RAM \end{cases} \quad (4.12)$$

Considering the fraction of effective precipitation (R_p) and irrigation (R_I), drainage accounts for the fractions of precipitation $P \cdot (1 - R_p)$ and irrigation $I \cdot (1 - R_I)$ not efficiently used by the soil-canopy unit. When the soil presents the maximum moisture it can hold, $SMD = 0$, the water that is supplied by irrigation or precipitation is drained (Eq. 4.13).

$$D = \begin{cases} P \cdot (1 - R_p) + I \cdot (1 - R_I), & SMD > 0 \\ P \cdot R_p + I \cdot R_I - SMD_{i-1} - ET, & SMD = 0 \end{cases} \quad (4.13)$$

Soil moisture depletion SMD is formulated in (Eq. 4.14), with a maximum $SMD=TAM$.

$$SMD = \begin{cases} SMD_{i-1} + ET - P \cdot R_p - I \cdot R_l, & 0 < SMD < TAM \\ TAM, & SMD > TAM \end{cases} \quad (4.14)$$

The model was calibrated through the energy consumption required to pump the drainage discharge from the study area (BXII) to the river. The calibration period covered a decade of study from 2003 to 2012, with a Nash–Sutcliffe coefficient $e_2 = 0.90$ between observed and estimated drainage discharge data.

4.2.3.5 Remote sensing global evapotranspiration product MOD16 ET

The MOD16 ET is a globally available algorithm for ET retrieval based on the Penman-Monteith equation (1965), produced at 8-days, monthly and annual time steps (freely accessible from <http://ntsg.umd.edu/project/mod16>). Firstly introduced by Mu *et al.* (2007a) based on a revision of the algorithm proposed by Cleugh *et al.* (2007), the algorithm resolves, during day-time, the crop and surface resistances to transpiration and evaporation flows to the atmosphere. In Mu *et al.* (2011) the algorithm was updated, considering the ET contribution during night-time, and other improvements on the vegetation cover fraction, stomatal conductance or aerodynamic conductance. The logic behind the MOD16 ET algorithm utilizes daily air pressure, air temperature, humidity and radiation as meteorological data, together with remote sensing data derived from MODIS, including land cover, LAI , f_{APAR} and α . In this study the monthly ET product has been used.

4.2.3.6 Validation of the PT-JPL-thermal ET

RS ET estimations derived from (i) the PT-JPL-thermal and (ii) the global ET product MOD16 were compared against WATEN ET calibrated data in the mixed-irrigation BXII from 2003 to 2012, where WATEN outputs were available. Monthly ET estimations as well as the average seasonal (monthly) and inter-annual ET dynamics were evaluated and compared. In this work ET has been expressed in mm/day because of the importance in this region of irrigation, field in which ET is usually given in mm/day. This value is calculated by dividing monthly ET by the number of days in the month. Table 4.12 illustrates the inputs and parameters required to derive ET from the three methods. Potential ET_p data series from PT-JPL-thermal and MOD16 were further compared against ET_p at the agro-climatic station at (BXII), Lebrija I.

Table 4.12 Model inputs and parameters required for *ET* retrieval from WATEN, PT-JPL-thermal and MOD16. *TAM*, total available moisture (mm month⁻¹); *RAM*, readily available moisture (mm month⁻¹); *R_b*, fraction of effective irrigation; *R_p*, fraction of effective precipitation; *ET*, evapotranspiration (mm month⁻¹); *D*, drainage (mm month⁻¹); *SMD*, soil moisture depletion (mm month⁻¹).

	WATEN	PT-JPL-thermal	MOD16
Inputs			
• RS data		<i>LAI/f_{APAR}</i> (MOD15A2) Broadband α (MCD43B3) <i>NDVI</i> (MOD13A2) <i>LST/Emis</i> (MOD11A2, MYD11A2)	<i>LAI/f_{APAR}</i> (MOD15A2) Broadband α (MOD43C1) <i>EVI</i> (MOD13A2) Land cover (MOD12Q1)
• Climatic data	Precipitation <i>P</i> Reference <i>ET_o</i>	Air temperature <i>T_{air}</i> Incoming shortwave radiation <i>R_{Sday}</i> [↓]	Meteorological reanalysis data GMAO: • Air temperature • Air pressure • Humidity • Radiation
• Other in-situ data	Sowing/harvesting dates Crop growth stages Crop coefficients Irrigation <i>I</i>		Biome-type look-up-table
Calibrated parameters	<i>TAM</i> , <i>RAM</i> <i>R_b</i> , <i>R_p</i>		
Outputs	<i>ET</i> , <i>D</i> , <i>SMD</i>	<i>ET</i>	<i>ET</i>

The performance of the PT-JPL-thermal and MOD16 *ET* models was evaluated through the Pearson correlation coefficient ρ (Eq. 4.15), *p* value or probability value, the Mean Absolute Error (*MAE*) (Eq. 4.16), the bias (Eq. 4.17) and the Root Mean Square error, (*RMSE*) (Eq. 4.18).

$$\rho_{x,y} = \frac{cov(x,y)}{\sigma_y \cdot \sigma_x} \quad (4.15)$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |y_i - x_i| \quad (4.16)$$

$$bias = \frac{1}{n} \sum_{i=1}^n (y_i - x_i) \quad (4.17)$$

$$RMSE = \sqrt{\frac{1}{n} \cdot \sum_{i=1}^n (y_i - x_i)^2} \quad (4.18)$$

Where cov (x,y) is the covariance between the observed *ET* values *x_i*, and the estimated RS *ET* values, *y_i*; σ_x and σ_y are the standard deviation of the variables, and (*y_i*−*x_i*) the estimated RS model error.

The coefficient of efficiency (e_2) (Nash and Sutcliffe, 1970), was used to determine the relative magnitude of the residual variance compared to the measured data variance (Moriasi *et al.*, 2007) (Eq. 4.19).

$$e_2 = 1 - \frac{\sum_{i=1}^n (y_i - x_i)^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \quad (4.19)$$

In addition, Theil's inequality decomposition was useful to break down the error in monthly ET rates into three different characteristic sources: bias (u_m), large values indicate a systematic error; variance (u_s), large values indicate large difference in the fluctuation of the series; covariance (u_c), low values indicate unsystematic errors due to randomness (Pindyck and Rubinfeld, 1998; Watson and Teelucksingh, 2002) (Eq. 4.20).

$$1 = u_m + u_s + u_c;$$

$$1 = \frac{n \cdot (\bar{y} - \bar{x})^2}{\sum_{i=1}^n (y_i - x_i)^2} + \frac{(n-1) \cdot (\sigma_y - \sigma_x)^2}{\sum_{i=1}^n (y_i - x_i)^2} + \frac{2(n-1) \cdot (1 - \rho_{x,y}) \cdot \sigma_y \cdot \sigma_x}{\sum_{i=1}^n (y_i - x_i)^2} \quad (4.20)$$

According to (Pindyck and Rubinfeld, 1998), Theil's inequality components distribution is close to optimum when the sum of all three components follows the ideal distribution $u_m \cong u_s \cong 0$ and $u_c \cong 1$; otherwise undesirable occurrences would point to a revision of the evaluated model.

4.2.3.7 Assessment of PT-JPL-thermal vs. MOD16 ET in the Doñana region

We compared the PT-JPL-thermal estimations against the globally available product MOD16 ET series over the Mediterranean region of Doñana (number of pairs $n_p=152640$, i.e. 1272 region-pixels in the 120 months-period from 2003 to 2012). ET annual values, inter-annual variability and seasonality patterns (monthly) were assessed and compared for different land uses (in Fig.1) and on a pixel basis.

Multiyear ET daily average values, normalized to the total average in the region (ET/ET_{av}) were used to assess the agreement between models in the spatial distribution of ET estimates. Multiyear average ET values were compared in terms of land use ($n_p = 906$ in the irrigated areas, $n_p = 366$ in the natural ecosystems).

Seasonal (monthly) and inter-annual patterns of ET over the study period were compared on a pixel basis by correlation coefficients ($n_p = 120$ i.e. 120 months per pixel, and $n_p = 10$ i.e. 10 years per pixel), which were further partitioned and analyzed by individual month and land cover class.

4.2.4 Results

4.2.4.1 Validation of the PT-JPL-thermal ET

The daily PT-JPL-thermal ET was aggregated into monthly estimates (mm/day), and compared against the in-situ calibrated hydrological model WATEN ET and MOD16 ET .

Annual ET values are shown in Fig. 4.14c. The 10-year average from 2003 to 2012 was 739 mm for PT-JPL-thermal and 352 mm for MOD16, which represented a 7% overestimation and 49% underestimation compared to WATEN ($ET=691$ mm) respectively. The ET time series resulting for the period 2003 to 2012 is shown in Fig. 4.14a. The average seasonality derived from the PT-JPL-thermal ET and WATEN ET , Fig. 4.14b, presented maximum ET values in June, whereas MOD16 ET maximum values were in April/May. The PT-JPL-thermal ET showed a high agreement with WATEN results one-month lagged.

Figure 4.14 a) Monthly ET (mm/day), b) average ET seasonality (mm/day), c) annual ET (mm/year) derived from WATEN, PT-JPL-thermal and MOD16 in the BXII for the period 2003-2012.

Fig. 4.15 shows the relationship between the PT-JPL-thermal and MOD16 monthly average ET values versus WATEN ET over the study period 2003 to 2012; Table 4.13 illustrates the performance of the models based on the estimators proposed (ρ coefficient, e_2 , MAE , bias and $RMSE$) for monthly and annual average values. In

general, the PT-JPL-thermal showed higher performance than MOD16. PT-JPL-thermal vs. WATEN correlation remarkably increased when considering 1-month lag between both models. Uncertainties derived from the WATEN-required inputs, particularly irrigation data taken indirectly from the transfer of water from the reservoirs for irrigation purposes (Moyano *et al.*, 2015) may explain this lag.

Table 4.13 Pearson correlation coefficient ρ , significant* at $p < 0.001$, the Nash-Sutcliffe e_2 , the Mean Absolute Error, MAE , the bias and the Root Mean Square error, $RMSE$ for the monthly ET and average climatology ET of PT-JPL-thermal and MOD16 vs. WATEN.

<i>Monthly ET</i>	ρ	e_2	<i>MAE Bias RMSE</i> (mm/day)		
PT-JPL-therm vs. WATEN	0.78*	0.59	0.74	0.13	0.9
PT-JPL-therm vs. WATEN _{1month-lag}	0.94*	0.87	0.39	0.13	0.51
MOD16 vs. WATEN	0.48*	-0.27	1.17	-0.92	1.58
<i>ET average seasonality</i>					
PT-JPL-therm vs. WATEN	0.83*	0.67	0.68	0.13	0.78
PT-JPL-therm vs. WATEN _{1month-lag}	0.99*	0.96	0.25	0.13	0.29
MOD16 vs. WATEN	0.65*	-0.28	1.15	-0.92	1.54

Figure 4.15 Scatterplot of monthly ET (mm/day) from PT-JPL-thermal and MOD16 versus WATEN ET in the mixed-irrigation BXII.

The Theil's inequality components distribution of the ET estimations derived from the PT-JPL-thermal and MOD16 ET models versus WATEN ET is illustrated in Table 4.14.

Table 4.14 Theil's inequality components distribution for monthly ET derived from PT-JPL-thermal and MOD16 vs. WATEN. Ideal Theil's inequality components distribution: $u_m \cong u_s \cong 0$ and $u_c \cong 1$.

<i>Monthly ET</i>	<i>Theil's inequality components</i>		
	u_m	u_s	u_c
PT-JPL-thermal vs. WATEN	0.02	0.02	0.96
MOD16 vs. WATEN	0.34	0.48	0.18

Potential evapotranspiration ET_p from MOD16 did however, significantly correlate with on-site ET_p at the agro-meteorological station Lebrija I ($\rho=0.98$, bias=0.2 mm/day); ET_p derived from PT-JPL-thermal also resulted in high correspondence with ET_p at Lebrija I ($\rho=0.99$, bias=0.17 mm/day) (Fig. 4.16).

Figure 4.16 a) Monthly ET_p (mm/day) derived from the agro-climatic station Lebrija I versus ET_p from the PT-JPL-thermal and MOD16 over 2003 to 2012. b) Average monthly correlation of ET_p (mm/day) from PT-JPL-thermal and MOD16 against ET_p at Lebrija I.

4.2.4.2 Assessment of PT-JPL-thermal vs. MOD16 ET in the Doñana region

For the period 2003-2012, the average evapotranspiration ET_{av} in the region, including irrigated areas and natural ecosystems, was estimated in 657 and 379 mm/year by the PT-JPL-thermal and MOD16 respectively; MOD16 reached a 58% of the PT-JPL-thermal estimated ET_{av} . The monthly average ET in the region, Fig. 4.17a, showed a low correlation ($\rho \cong 0.48$) and a large bias=-23.6 mm between models for a number of pairs $n_p = 120$ months. At annual time-scale for a $n_p = 10$ years, the agreement between models increased ($\rho \cong 0.94$, $p < 0.001$) and the bias remained large, Fig. 4.17b.

Figure 4.17 a) Region-averaged ET_{av} (mm/day), b) region-averaged ET_{av} (mm/year) derived from the PT-JPL-thermal and MOD16 in the study region (irrigated areas plus natural ecosystems), from 2003 to 2012.

In the Doñana region, MOD16 showed a systematic negative bias with respect to the PT-JPL-thermal estimations for all the land cover classes. In addition, the timing of the peak intra-annual ET values was non-coincident between models, Fig.4.18. The mixed-irrigation lands, Figs. 4.18a and 4.18b, presented maximum ET values in summer (June to August) for the PT-JPL-thermal, and spring (April to May) for MOD16; the rice fields presented maximum ET values from July to August for both the PT-JPL-thermal and MOD16, Fig. 4.18c. In the natural ecosystems, the PT-JPL-thermal showed maximum ET values in May for the wetland, Fig. 4.18d, in June for the shrubland, Fig. 4.18e, and July for the coniferous forest, Fig. 4.18f, while MOD16 detected maximum ET values in April for the three natural ecosystems.

Figure 4.18 PT-JPL-thermal and MOD16 ET seasonality over the period 2003-2012: a to c) in the irrigated areas (rice fields and mixed-irrigated lands), d to f) in the natural ecosystems (wetland, shrubland and coniferous forest).

The spatial patterns of the normalized ET values (ET/ET_{av}), Fig. 4.19, showed a high agreement between models, both depicting the areas with higher and lower ET rates accordingly, except for the wetland. Both models identified the higher normalized ET values in the rice fields and coniferous forests, and those close to the region average ET_{av} in the mixed-irrigation areas and shrubland. However, it was found a significant disagreement in the ET for the wetland: it resulted well above and below the ET_{av} in the estimations derived from PT-JPL-thermal and MOD16 respectively.

Figure 4.19 Normalized ET values. ET/ET_{av} , where ET is the multiyear average ET per pixel and ET_{av} is the average ET within the region over the period 2003-2012. a) PT-JPL-thermal $ET_{av} = 1.81$ mm/day, b) MOD16 $ET_{av} = 1.03$ mm/day.

The scatterplots in figures 4.20a and 4.20b show the relationship between the multiyear daily average ET estimations derived from the PT-JPL-thermal and MOD16 over the period from 2003 to 2012, differentiating by irrigated areas and natural ecosystems. The correlation was found significant in the irrigated areas, with $\rho=0.74$ ($p<0.001$) and a bias=-0.73 mm/day. In contrast, the correlation values were low in the natural ecosystems, with $\rho=0.17$ ($p<0.01$) and a bias=-0.90 mm/day, except for the shrubland, which showed a correlation value $\rho=0.68$ ($p<0.001$) and a bias of -0.59 mm/day.

Figure 4.20 a) PT-JPL-thermal vs. MOD16 multiyear average ET estimations (mm/day) in the irrigated areas and b) the same for natural ecosystems.

Figs. 4.21a and 4.21b show the temporal correlation values between model estimations at seasonal (months) and inter-annual scales. Higher correlation values were found in the inter-annual ET dynamics compared to the seasonal correlations.

Figure 4.21 Temporal correlation between PT-JPL-thermal and MOD16 for a) seasonal ($n_p = 120$, 120 months per pixel) and b) inter-annual ($n_p = 10$, 10 years per pixel).

The scatterplots in figure 4.22 show the relationships between the PT-JPL-thermal and MOD16 *ET* estimations for all the land covers grouped for each month ($n_p = 12720$ i.e. 1272 pixels in 10 years). Significantly higher correlation values were found in the summer months (i.e. July August and September) than in the period from October to March, while the rest of the months did not show any significant correlation.

Figure 4.22 Monthly *ET* (mm/month) from PT-JPL-thermal vs. MOD16 in the study region (irrigated areas plus natural ecosystems), number of pairs $n_p = 12720$ (1272 region-pixels in 10 years from 2003-2012).

This information is complemented by Figs. 4.23a and 4.23b, which show specific correlation values for each month and land cover class.

A high significant correlation was found in the irrigated areas during the months of maximum water demand, Fig. 4.23a. In the natural ecosystems, Fig 4.23b, it was found a non-significant correlation. Particularly for the wetland, the correlation coefficient was $\rho=0.07$ with $p=0.25$; for the coniferous forests $\rho=-0.04$ with $p=0.86$. However, a significant correlation was observed in the shrubland over spring and summer months ($\rho>0.7$).

Figure 4.23 Correlation coefficients of the PT-JPL-thermal vs. MOD16 *ET* monthly patterns over 2003 to 2012 for a) the irrigated areas and b) the natural ecosystems.

4.2.5 Discussion

4.2.5.1 Validation of the PT-JPL-thermal *ET*

The *ET* derived from the PT-JPL-thermal showed, for all the estimators proposed (Table 4.13), a better performance than the estimated *ET* from MOD16, in which the high bias obtained indicates a significant underestimation of *ET* rates. Moreover, significant differences were observed in the *ET* dynamics between models, with non-coincident timing of the peak annual values.

The PT-JPL-thermal *ET* dynamics at monthly scale (Table 4.13) showed a good agreement with WATEN *ET*. The amount of variance explained and the e_2 coefficient indicate that the PT-JPL-thermal model is able to accurately capture the *ET* dynamics. On the other hand, MOD16 e_2 negative values suggest a high variance in the residuals which, together with the high values of the calculated errors, indicate a low capability for reproducing the WATEN *ET* dynamics. In addition, the Theil's distribution components of the *ET* estimations (Table 4.14) obtained with the PT-JPL-thermal were

close to ideal, with a low bias, a well represented variance and non-systematic residual errors in *ET* estimations. For MOD16, the Theil's inequality components distribution showed a poor model performance under our Mediterranean conditions.

When considering the average seasonality in the *ET* dynamics (Table 4.13), the PT-JPL-thermal estimates showed better results than the *ET* dynamics at monthly scale, with higher amount of variance explained and smaller errors. On the other hand, the WATEN *ET* seasonality was not accurately represented by MOD16, which showed a similar e_2 coefficient and error values than those obtained at monthly scale over the whole study period.

Since potential *ET* values estimated by Penman-Monteith (used in MOD16) and Priestley Taylor (PT-JPL-thermal) were similar (Fig. 4.16), it could be assumed that the disagreement between models resulted in the downscaling process from potential to actual *ET*. MOD16 considers soil evaporation fluxes as a function of relative humidity (*RH*) and vapor pressure deficit (*VPD*); although this criterion may work for non-irrigated areas, it may lose reliability in irrigated areas where the water applied to the crop is not reflected in the *VPD* alone (Yilmaz *et al.*, 2014). High values of *VPD* may reflect the surrounding arid conditions, but do not take into account the real values of water availability. In addition, MOD16 considers the surface of the soil covered by water to be zero when *RH* is less than 70%; *RH* records were below 70% over the irrigation season from 2003 to 2012 at the agro-climatic station Lebrija I and in consequence, MOD16 assumed the wet surface fraction as non-existent, leading to an underestimation of *ET*. Likewise, Biggs *et al.* (2016) found the evaporative fraction from the irrigated cotton (the major cultivated crop in the mixed-irrigation BXII) to be underestimated in a 67%. The significant correlation between the PT-JPL-thermal and WATEN *ET* estimations proves that the use of the thermal inertia concept as a proxy indicator of moisture status, together with the re-formulation of the outgoing longwave radiation, makes it possible to reproduce the dynamics of *ET* under our Mediterranean conditions in a more accurate manner than the *VPD* alone.

4.2.5.2 Assessment of PT-JPL-thermal vs. MOD16 *ET* in the Doñana region

In the whole Doñana region, MOD16 estimations were also significantly lower than the PT-JPL-thermal *ET* values, Figs. 4.17. On the other hand, a high agreement between models *ET* estimation was found in the whole region inter-annual dynamics, Fig. 4.17b, and at pixel level, Fig. 9b, with ρ values around 0.8 in most of the pixels. As previously

found by Mu *et al.* (2007b), although *VPD* alone may fail to capture the seasonality of water stress in some areas, Fig. 4.21a, the inter-annual variability of water stress could be captured by *VPD* alone in most areas, Fig. 4.21b, indicating the adequation of this approach for inter-annual global studies (Mu *et al.*, 2007b).

The PT-JPL-thermal *ET* estimations reasonably approached documented *ET* rates in the region per land cover class, thereafter detailed. The mixed-irrigation areas were found to evapotranspire 4-5 mm/day in summer by the PT-JPL-thermal, Fig. 4.18a and 4.18b, in accordance with the on-site calibrated WATEN *ET* estimations in the mixed-irrigation BXII. In the rice fields, irrigation supply is documented to be 6.3 mm/day on average, in a 5-months crop-cycle (JdA, 2007), reasonably approached by the PT-JPL-thermal *ET* estimations, Fig. 4.18c. Previous studies (Drexler *et al.*, 2008) in Mediterranean-climate wetlands showed similar *ET* average values than those estimated by the PT-JPL-thermal from May to October (i.e. 6 mm/day with σ =1.9 mm/day vs. 4 mm/day), indicating that MOD16 may be underestimating evaporative fluxes, Fig. 4.18d. Penatti *et al.* (2015) obtained similar results in the world's largest wetland (Pantanal) with a significant *ET* underestimation after winter and spring rainfall-periods. For the shrubland, Fig. 4.18e, MOD16 might probably underestimate *ET* due to be a land use characterized as poorly vegetated surface, as in previous findings in the Central Great Plains of the United States (Velpuri *et al.*, 2013). Although MOD16 has been documented to overestimate *ET* in forested areas over the Northeast Asia monsoon region (Jang *et al.*, 2013; Hu *et al.*, 2015), it was found to underestimate *ET* for coniferous forests under Mediterranean conditions, Fig. 4.18f.

Intra-annual dynamics of the PT-JPL-thermal *ET* were coincident with on-site irrigation management and natural patterns correspondent to the study-region land uses, whereas MOD16 *ET* presented some inconsistencies. The two mixed-irrigation areas (BXII and left bank), showed maximum MOD16 *ET* values in April, contrary to the irrigation-patterns in the region (June to August) which were more accurately identified by the PT-JPL-thermal, Fig. 4.18a and Fig. 4.18b. For the rice fields, both MOD16 and the PT-JPL-thermal identified maximum *ET* values in July and August, Fig. 4.18c, in accordance with the rice fields' management in the region: a 5-months cultivation-cycle from May to September, after which plots are drained and rice is harvested in October (JdA, 2007). In the natural ecosystems, maximum PT-JPL-thermal *ET* fluxes were observed when the evaporative demand from the atmosphere ET_p was high, and when

water was available and easily accessible. Thus, the natural ecosystems showed different *ET* patterns depending on their capability to access water. The wetland *ET* dynamics were accurately captured by the PT-JPL-thermal *ET* estimations, Fig. 4.18d, with highest *ET* fluxes in April-May when water is available after rainfall and vegetation sprouts (Ontillera and González-Nóvoa, undated). Our results match *ET* intra-annual dynamics previously documented by Drexler *et al.* (2008) in a similar Mediterranean-climate wetland in the Sacramento-San Joaquin Delta, in California. For the shrubland, Fig. 4.18e, maximum rates were observed later in spring (i.e. around June), coincident with the spring green-up period, which is supported by deep infiltration of winter and early spring precipitation, as previously observed by Nagler *et al.* (2007) in semiarid shrublands. In the coniferous forest, Fig. 4.18f, maximum *ET* values occurred later in summer (i.e. July-August) coincident with maximum ET_p values and showing their root capability to access deeper soil moisture layers (Garcia *et al.*, 2009). On the contrary, MOD16 showed maximum *ET* values in April and lowest *ET* values in July for the three ecosystems equally, since this model relies on large-scale meteorological variables to estimate *ET* and apparently, is not able to capture ecosystem differences. In addition, the lowest *ET* values identified by MOD16 in July indicate the low capability of this model to assess *ET* fluxes in dry atmospheres with enough soil moisture availability (Mu *et al.*, 2007a). Since MOD16 bases the soil evaporation on *RH* and *VPD* alone, it does not take into account the availability of water in deep layers, accessible for the shrublands and forests' roots during part of the summer. This is especially important in the Doñana region because of the presence of the aquifer Almonte-Marismas on which the region rests, assuring water availability for some natural vegetation.

The *ET* spatial patterns derived from both models estimations clearly depict the land use distribution in the region, with a significant agreement between models except in the wetland (Fig. 4.19), where MOD16 *ET* values were lower than the average values in the region, while PT-JPL-thermal *ET* values were higher. MOD16 uses a land cover map for parameterization and, therefore, A differentiation of land uses was expected; the fact that the land uses map does not include a wetland class may partially explain the low *ET* rates in this area. In addition, the *RH* criteria used in MOD16 (Mu *et al.*, 2011) results in an erroneous elimination of the surface water cover fraction from April to October in the study region (*RH* below 70%). On the other hand, the PT-JPL-thermal is able to

capture the distinct moisture dynamics among land cover classes accurately producing spatially consistent values within land uses and identifying large differences among them (Fig. 4.19). This indicates that the physical concept of thermal inertia is applicable to different patterns of moisture availability, such as areas with free water surfaces, irrigated crops and natural vegetation extracting the water from deep layers.

Within land uses, the correlation of multiyear average *ET* between models at the pixel level was relatively high ($\rho=0.74$) in the irrigated areas, Fig. 4.20a, while in the natural ecosystems the agreement was much lower ($\rho=0.17$), Fig. 4.20b. In the irrigated areas, despite the *ET* underestimation by MOD16, both methods seem to differentiate those pixels with more and less evaporation accordingly, Fig. 4.20a. However, the two models do not coincide in identifying the pixels with higher and lower *ET* values in the natural ecosystems, especially in the wetland, Fig. 4.20b. The availability of water for natural ecosystems due to the underlying Almonte-Marismas aquifer might be better captured by the thermal inertia approach used by the PT-JPL-thermal than with the *HR* and *VPD* approach used by MOD16. In addition, higher correlation values ($\rho>0.80$) were found in the months of maximum water demand, i.e. from July to September (Fig. 4.22). In particular, the rice fields and mixed-irrigation left bank showed the highest agreement in these months (Fig. 4.23), in contrast to the natural ecosystems. A possible explanation is that the land cover product used to constraint *ET* values depending on land use is correctly assigned to the shrublands and fails in the coniferous forest; thus a wrong parameter assignation in the forest may be the reason why PT-JPL-thermal and MOD16 present such low *ET* correlation values.

4.2.6 Conclusions

We compared two evapotranspiration models in natural ecosystems and irrigated lands within the UNESCO protected Doñana Mediterranean region over the period from 2003 to 2012. We validated the *ET* estimations obtained from the thermally modified PT-JPL model (PT-JPL-thermal), that introduces land surface temperature (*LST*) with a thermal inertia approach as a proxy to the soil moisture status, against the on-site calibrated hydrological model WATEN, and compared inter and intra-annual *ET* patterns with the globally available MOD16 *ET* product. The PT-JPL-thermal was found to reasonably reproduce the *ET* dynamics under our Mediterranean conditions ($\rho=0.78$, $\rho_{1\text{-month lag}}=0.94$), in contrast to MOD16 *ET* estimates, which pointed to a poor model performance in the region. We found that MOD16 would allow (i) to easily identify land uses with

lowest and largest water demands and (ii) to assess inter-annual variability of *ET* in water-limited regions. However, the large negative bias (58% underestimation) found on MOD16 *ET* estimations in the evaluated land uses (irrigated areas plus natural ecosystems: wetland, shrubland, coniferous forest), would not allow MOD16 to approach the *ET* quantification under water-limited conditions. The PT-JPL-thermal reasonably approached expected *ET* rates in the region, revealing well-differentiated and coherent spatio-temporal patterns among the evaluated land uses, and pointing to the PT-JPL-thermal as an alternative proxy to *ET* estimations in water-limited regions. This study has proved that the use of the thermal inertia concept as a proxy indicator of soil moisture status, together with the re-formulation of the outgoing longwave radiation, is capable to reproduce *ET* at regional level in semiarid environments, requiring only air temperature and incoming solar radiation from climatic databases apart from standard satellites-products freely available for *ET* estimations.

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4.3 Study III. Increasing competition for water between crops and natural ecosystems as the land dries: a case study in the Doñana region

Abstract. In many areas of the world, natural ecosystems and crops compete for the same water sources; this competition increases as regions dry. To understand stresses on natural ecosystems and agriculture, water use and demand for both must be quantified to identify tipping points in water availability and demand. The objective of this research was to understand the changes in the water use by vegetation that the World Heritage UNESCO Doñana region has experienced for the past decades. We track changes in the spatial and temporal characteristics of water use and demand through a thermally-modified global *ET* remote sensing model (PT-JPL-thermal), a sound remote sensing model for detecting *ET* in arid environments. Station-measured precipitation (*P*) significantly decreased overall from 2011-2016. *ET* was highly correlated with *P* only in the wetlands, and to a much less extent in the forests and croplands, suggesting that the wetlands may be most susceptible to overall drying, though the whole region is susceptible. However, to exacerbate the situation, we found that *ET* increased in the intensified agriculture and rice fields, pointing to a greater diversion of water to crops when water supply has been dwindling. These results help to inform water management decisions and consequences when balancing regional demands for food production and ecological sustainability.

4.3.1 Introduction

The growing increase in the world's population and food demand impose stresses to natural ecosystems, many of which require access to the same water resources as agricultural lands (Tanentzap *et al.*, 2015; Muller *et al.*, 2017). One of the greatest challenges of our time is to feed more than 9 billion people by 2050 while maintaining the integrity of natural ecosystems in a context of increasing climate extremes (Alexandratos and Bruinsma, 2012). Increasing extremes in precipitation and temperature are threatening crop production and food security (Mushtaq *et al.*, 2015), affecting the functionality of ecosystems worldwide (Scholes, 2016).

A prime example of this is the Mediterranean region, one of the most prominent responsive regions to climate change (Giorgi, 2006), where biodiversity and ecosystem functioning are already heavily threatened (Rodriguez-Ramirez *et al.*, 2017). The Iberian Peninsula is expected to be amongst the most affected areas by severe droughts

(Diffenbaugh *et al.*, 2007), prone to suffer significant reductions of groundwater recharge by the end of the 21st century, particularly pronounced in the river basins of southern Spain (Kovats *et al.*, 2014) where irrigated agriculture amounts 80% of the total extracted water (Minacapilli *et al.*, 2009). Since natural ecosystems are affected by irrigation consumption, irrigation restrictions are foreseen to occur in more environmentally-focused future scenarios (Henriques *et al.*, 2008); there is a need to improve our knowledge on ecosystems responses to future environmental conditions (Rodríguez-Ramírez *et al.*, 2017).

Wetlands are particularly affected by land uses conversion to agriculture, accounting for as much as 71% of wetlands in Europe that may have disappeared since the beginning of the last century (Kingsford *et al.*, 2016). In the Guadalquivir River basin in southern Spain, the water consumption is expected to increase up to a 20% by 2050 (Chavez-Jimenez *et al.*, 2015) which may lead to a poor ecological conservation of the associated natural ecosystems (García De Jalón *et al.*, 2014). A significant case is the Doñana Biosphere reserve located at the mouth of the Guadalquivir River basin and included in the international Ramsar Convention for wetlands conservation.

The Doñana wetlands depend on both groundwater and surface water; in the last years streams flow rates have roughly halved (Green *et al.*, 2017a) and groundwater over-exploitation has lowered the water table in more than 6 m, threatening the functioning of the Doñana ecosystems (Green *et al.*, 2017b), including wetlands, shrublands and coniferous forests. The World Heritage Committee (UNESCO, 2017) has recently urged to tackle the problem of illegal water abstraction to avoid the inscription of Doñana into the List of World Heritage in Danger. Further monitoring and modelling the hydrological cycle in the region is key to reverse these trends by adjusting water demands and inform policy makers (UNESCO, 2017).

Evapotranspiration (*ET*) is a central process in the hydrological cycle, returning about 60% of annual precipitation to the atmosphere and being responsible for the distribution of water and energy on land surfaces, particularly in semiarid regions (Zou *et al.*, 2017). Moreover, *ET* can affect precipitation and have important implications on the intensity and duration of heat waves (Jung *et al.*, 2010). Accurate spatially distributed estimates of *ET* allow to discretize water consumption from crops and vegetation (Zou *et al.*, 2017), and to open up new avenues in the management of water resources by integrating

blue (surface and groundwater) and green (rainfall-based) sources for sustainable development (Hoff *et al.*, 2010; Velpuri *et al.*, 2013).

Evapotranspiration at specific locations can be estimated by using methods such as lysimeters, Bowen-ratio or eddy covariance amongst others (Allen *et al.*, 2011). For *ET* estimations at large-scales remote sensing (RS) methods are preferable, offering wide spatial coverage (Zou *et al.*, 2017). Diagnostic or historical Land Surface Models (LSM) using RS to prescribe vegetation and other surface variables can provide spatially distributed fluxes and fast updating of the land surface (Olivoso *et al.*, 1999; Xu *et al.*, 2014). These models need limited a priori data of soil and vegetation parameters to estimate *ET* and can rely on RS-land surface temperature (*LST*) as a proxy to the surface moisture status (Yilmaz *et al.*, 2014). This is the case of the thermally-modified version of the Priestley-Taylor Jet Propulsion Laboratory (PT-JPL), which reduces potential *ET* based on novel ecophysiological constraints to land-atmosphere water fluxes (Fisher *et al.*, 2008), avoiding the need of soil moisture content, stomatal resistances and wind speed data. García *et al.* (2013) proposed a modification of the PT-JPL model (PT-JPL-thermal) with a thermal inertia approach as a proxy to the soil moisture status, performing well in drylands under Mediterranean and monsoonal conditions at Eddy Covariance (EC) flux sites. The PT-JPL-thermal model has been recently validated for first time at regional scale with modelled net radiation at the Mediterranean semiarid region of Doñana (Moyano *et al.*, under revisión, 2018), reasonably approaching documented *ET* rates and revealing well-differentiated and coherent spatio-temporal patterns.

Direct observational evidences of *ET* trends are still lacking, although recent studies point to the largest declines on *ET* trend in those regions where *ET* is limited by moisture. When *ET* becomes more and more supply-limited in the long term, terrestrial productivity and terrestrial carbon sink are reduced, accelerating the land-surface warming (Jung *et al.*, 2010). The identification of hot-spots or areas where the water used by natural ecosystems is declining independently of rainfall patterns, or sites where the water use is significantly increasing due to farming intensification can benefit society by helping managers to allocate water resources. At present, research efforts are intensified towards a comprehensive analysis of changes on *ET* trends and associated driving forces (Zhang *et al.*, 2016; Jin *et al.*, 2017; Mo *et al.*, 2017), some of them using thermal infrared data to track surface moisture status (Verstraeten *et al.*, 2006;

Minacapilli *et al.*, 2009; García *et al.*, 2013; Qin *et al.*, 2013; Autovino *et al.*, 2016; Leng *et al.*, 2017) overcoming the need of water vapor data and field site calibrations for the assessment of water dynamics. The analysis of the historical values of water evapo-transpired by crops and ecosystems, the changes produced over time and their relation to changes in the climate can help to understand the resilience of vegetation and to establish safe operating spaces (Green *et al.*, 2017a).

The overall goal of this study is to quantify the historical *ET* dynamics in the Doñana region over the period from 2003 to 2016, where natural wetlands and irrigated crops compete for the use of water resources and where the number of conflicts between environment conservation and economic development has significantly increased in the last decade (Martín-López *et al.*, 2011). We specifically aimed to identify hotspots of increasing or decreasing *ET* rates, and the underlying driving forces.

To achieve this goal we set up three specific objectives:

- To analyse spatio-temporal water use from daily to annual time scales from 2003 to 2016, at 1 km pixel resolution in the Doñana region, including croplands and natural ecosystems (wetlands, shrublands and coniferous forests).
- To identify pluri-annual periods of increasing or decreasing water use in Doñana natural ecosystems, assessing the precipitation, greening, and atmospheric demand changes as the explicative variables for the trends.

4.3.2 Study area

The study area covers the Doñana National Park (54251 ha) and natural Park (53835 ha), including the surrounding areas over the aquifer Almonte-Marismas in Andalusia. These areas include natural ecosystems within the Park, differentiating wetlands, shrublands and coniferous forests, and agricultural lands, particularly rice fields (García De Jalón *et al.*, 2014) on the right and left bank of the Guadalquivir river and mixed-irrigated croplands established in ancient river marshes. These marshes, originally extended over 150000 ha, have greatly evolved over the history (García Novo and Marín Cabrera, 2006), being reduced to the actual 30000 ha of seasonal marshes (fed by streams and rainfall) and 3000 ha of temporary dune ponds (fed by the aquifer) in the National Park. Since the 60s, the remaining ancient marshes were converted into arable land, causing a deep landscape change (Martín-López *et al.*, 2011) and defining the actual landscape of the region. To counteract this trend, it was declared a National Park

in 1969, included in the Ramsar Convention as one of the largest wetlands in Europe (Green *et al.*, 2017b) and designated a World Heritage Site by UNESCO in 1995. The National Park has also been buffered by a Natural Park which entered the endangered Montreux Record of Ramsar sites in 1990 (Serrano *et al.*, 2016). Conflicts have increased between the environment conservation and economic development in the Park (García Novo and Marín Cabrera, 2006), leading to a drawdown of the water-table in the aquifer Almonte-Marismas on which the Doñana region rests (2409 km²) and to a partial loss of the seasonal ponds (Guardiola-Albert and Jackson, 2011). Additionally, high concentrations of nitrates from agrarian origin in the aquifer (Oliás *et al.*, 2008) has led to many of the croplands, rice fields and wetlands in the area designated as nitrate vulnerable zones (CHG, 2015) under the European Commission nitrates directive (EU, 1991). Nowadays, about 11250 ha are under irrigation, of which WWF (2016) estimates a 15% may be under irregular status. If the actual management of the aquifer is sustained in-time, the sustainability of its associated ecosystems would be compromised (CHG, 2017).

4.3.3 Materials and methods

4.3.3.1 Remote sensing dataset

Multiple remote sensing observations were acquired from the Moderate Resolution Imaging Spectroradiometer (MODIS), using sensors from both Aqua and Terra satellites. Satellite data were used in combination with *in situ* meteorological data (air temperature and radiation) as inputs for the PT-JPL-thermal model. MODIS land products were retrieved from The Earth Observing System Data and Information System (EOSDIS), a core capability in National Aeronautics Space Administration (NASA) Earth Science Data Systems Program. All the selected MODIS products (version 5) were acquired at 1km pixel resolution for the 2003-2016 study period. The temporal resolution of the data sets were: (1) daily for Land Surface Temperature (*LST*) and Emissivity (*Emis*) from MOD11A2 and MYD11A2; (2) 8-day-composites of Leaf Area Index (*LAI*) and Fraction of Photosynthetically Active Radiation (*f_{APAR}*) from MOD15A2, broadband surface albedo (α) acquired from MCD43B3 and (3) 16-day-composites of Normalized Difference Vegetation Index (*NDVI*) retrieved from MOD13A2. For the 8 and 16 day-composites variables, the same value was used for the entire period.

4.3.3.2 Meteorological data

Meteorological data were obtained from the agro-climatic station Lebrija I (36.98°N lat., 6.13°W long., <https://www.juntadeandalucia.es/agriculturaypesca/ifapa/ria/>), a station site of the Agroclimatic Information Network of Andalusia (RIAA in Spanish). This station is controlled by a CR10X datalogger (Campbell Scientific) with sensors to measure T_{air} (T_{max} , T_{min} and T_{mean}), relative humidity RH (RH_{max} , RH_{min} , RH_{mean}), solar radiation R_s , precipitation P , wind speed and direction and reference evapotranspiration ET_o , transferred by GSM modems for quality control and data validation (Estévez *et al.*, 2011)

4.3.3.3 Land use maps

Land use maps were retrieved from the 2013 update Land Cover and Use Information System of Spain (SIOSE) database in the Doñana region. <http://www.juntadeandalucia.es/medioambiente/site/rediam/>. SIOSE is accessible at 1:10000 scale, European Terrestrial Reference System 1989 (ETRS89) under the European Directive INSPIRE (2007/2/CE) requirements.

4.3.3.4 Remote sensing ET based on a thermal and optical RS model

The PT-JPL-thermal model is described in García *et al.* (2013), based on the PT-JPL model of Fisher *et al.* (2008). In this work, the PT-JPL-thermal model was spatially distributed over the study area for a 14 years-period at a daily time-scale, following model validation in the semiarid region of Doñana and surrounding irrigated areas (Moyano *et al.*, under revisión, 2018).

4.3.3.5 Spatio-temporal ET dynamics in the Doñana region

We calculated daily ET derived from the PT-JPL-thermal model and the ratio of ET to potential rates i.e. the Water Deficit Index (WDI) (Moran *et al.*, 1994) for assessing the seasonal water use (Köksal, 2008) and availability (Lorenz *et al.*, 2016) in the region. WDI is herein computed as ET/ET_p , where low values of WDI would imply high water deficit indexes and vice versa. We aggregated daily ET and WDI (ET/ET_p) model outputs into monthly and annual data for each evaluated land cover class. The spatial means of ET and WDI were computed for each land cover (irrigated areas: mixed-irrigation BXII, mixed-irrigation left bank, rice-right and rice-left, and natural ecosystems: wetland, shrubland and coniferous forest) on a monthly basis from 2003 to 2016.

The standardized anomalies of ET and P (Dabernig *et al.*, 2017) were calculated for each land cover class as in Eq. 4.21 and Eq. 4.22:

$$STDA_{ET_i} = \frac{ET_i - \overline{ET}}{\sigma_{ET}} \quad (4.21)$$

$$STDA_{P_i} = \frac{P_i - \bar{P}}{\sigma_P} \quad (4.22)$$

Where ET_i and P_i are the annual ET and P values for year i , $\overline{ET}$ and $\bar{P}$ are annual means, and σ_{ET} and σ_P are standard deviations of the time-series.

The cumulative distribution function of the standardized ET and P anomalies $\Phi_{0,1}(STDA_{ET,P})$ was used to indicate the associated probability levels of each variable. $STDA$ values were considered anomalous when $\Phi_{0,1}(STDA_{ET,P}) > 0.95$ probability level. The same approach, using precipitation, was used to identify dry and humid years.

4.3.3.6 Pluri-annual ET periods and trends in the Doñana natural ecosystems

In the Doñana National Park, where natural ecosystems (wetland, shrubland and coniferous forest) are dependent on precipitation, unitary cumulative deviations from the mean, $CUDM_{ET}$ and $CUDM_P$ (Eq. 4.23 and 4.24) were used to detect the presence of pluri-annual periods of increasing or decreasing P and ET patterns (Archer and Fowler, 2004). These were identified by pronounced positive deviations from the mean (i.e. steeply rising slopes) or vice versa.

$$CUDM_{ET_i} = (ET_i / \overline{ET}_{i=1}^n - 1) + CUDM_{ET_{i-1}} \quad (4.23)$$

$$CUDM_{P_i} = (P_i / \bar{P}_{i=1}^n - 1) + CUDM_{P_{i-1}} \quad (4.24)$$

A linear regression model was fitted to detect ET annual trend values within the natural ecosystems from 2003 to 2016.

The double mass curve is widely used for long-term trend test of hydro-meteorological data, allowing to estimate the degree of proportionality between variables (Gao *et al.*, 2013; Odongo *et al.*, 2015). For the Doñana wetland in particular, a double-mass curve permitted to evaluate whether the ET trends were in agreement with changes in water supply (P), atmospheric water demand (ET_p) or vegetation greenness changes ($NDVI$) as explicative variables for the trends. As long as the ET does not change in time, the double mass curve produces a straight line, an inflexion in the curve is indicative of changes in the trend.

4.3.4 Results

4.3.4.1 Spatio-temporal *ET* dynamics in the Doñana region

The daily *ET* spatio-temporal series from the PT-JPL-thermal clearly revealed well differentiated and coherent spatio-temporal patterns among the evaluated land cover classes.

Fig. 4.24 illustrates the estimated *ET* and *WDI* (ET/ET_p) monthly values over 2003-2016, and except for the coniferous forests, that have access to the water table and can cope with drought, the most significant differences among the Doñana natural ecosystems (wetland and shrubland) and the irrigated areas were found in the driest year of the series, 2005.

For the irrigated areas (Fig. 4.24a), maximum values of *ET* were observed during the irrigation season (June to September), with peak average values in July for both the rice fields (198 mm/month) and mixed-irrigation areas (125 mm/month). Maximum *ET* reductions were registered from 2006 to 2008, mostly pronounced in 2008. In 2008, *ET* for the most-evaporative month, July, suffered a 30% and a 50% reduction in the mixed-irrigation areas and rice fields respectively. Maximum values of *WDI* (lower deficit) were also found from June to September over the study period. For the rice fields, *WDI* values showed lower deficits in the summer months (>0.8) except for years 2006 to 2008, where *WDI* descended below 0.5 (higher deficit). For the mixed-irrigation areas, *WDI* descended from an average value $WDI=0.5$ over the study period to a low value (higher deficit) $WDI=0.35$ in July 2008.

For natural ecosystems (Fig. 4.24b), maximum values of average monthly *ET* occurred in May for the wetland (109 mm/month), July for the shrubland (98 mm/month) and July for the coniferous forest (180 mm/month). *ET* suffered a marked reduction during the most-evaporative months of 2005 (55% in the wetland, 27% in the shrubland). Minimum values of *WDI* occurred from June to September over the study period. *WDI* values were notoriously lower (higher deficit) in years 2005 and 2012 for the wetland and the shrubland, with maximum monthly reductions in 2005. For the wetland, *WDI* values in the most-evaporative month of May were, on average, above $WDI=0.5$ except for years 2005 and 2012, where *WDI* descended below 0.25. For the shrubland, the drop was smoother in the most-evaporative month, July, from an average $WDI=0.4$ to $WDI<0.29$ in July 2005.

Figure 4.24 ET , precipitation P (mm/month) and monthly WDI (ET/ET_p) derived from the PT-JPL-thermal 2003-2016 for a) the irrigated areas (mixed-irrigation lands and rice fields) and b) the Doñana natural ecosystems (coniferous forest, wetland and shrubland). Due to rice-right/rice-left and mixed-irrigation BXII/mixed-irrigation left bank similarities, only rice-right and mixed-irrigation BXII are illustrated in a).

Among years, the coefficient of variation CV for ET in the evaluated land cover classes fluctuated from a minimum 0.08 in the coniferous forest to a maximum $CV=0.29$ in the wetland (Fig. 4.25). For the irrigated areas, minimum values of ET were registered in years 2007 and 2008 for both the rice fields (605 mm/year) and mixed-irrigation sites (530 mm/year), over an average annual value of 900 mm/year and 620 mm/year for the period 2003-2016 respectively. WDI values in the rice fields were particularly reduced in years 2007 and 2008 (0.38 over an average $WDI=0.47$). In the natural ecosystems, average annual values of ET reached 680 mm/year in the wetland, 620 mm/year in the shrubland and 1020 mm/year in the coniferous forest over the period 2003-2016.

Minimum values of ET were registered in 2005 for both the wetland (430 mm/year) and shrubland (450 mm/year), and from 2012 to 2016 (507 mm/year for the wetland; 550 mm/year for the shrubland). WDI was markedly reduced in 2005 (0.25 for the wetland, 0.24 for the shrubland, 0.49 for the coniferous forest), where precipitation reached minimum values in the series (240 mm/year), and from 2012 to 2016 (<0.33 for the wetland and the shrubland) over an average value of 0.43 and 0.35 for the wetland and shrubland, respectively, over the period 2003-2016.

Figure 4.25 Annual average values of precipitation P , ET (mm/year) and WDI for the irrigated areas and natural ecosystems derived from the PT-JPL-thermal over 2003-2016. Results from ET in the mixed-irrigation left bank and rice-left bank are not included due to the high similarities with mixed-irrigation BXII and rice-right respectively. The red square accounts for precipitation P and ET patterns in the driest year of the series, 2005.

Fig. 4.26 illustrates the mean annual ET values for the region over the entire period 2003-2016. Spatial differences among 2005 (dry year, $P=241$ mm) where ET reductions were very pronounced in the natural ecosystems, 2007 where ET reductions were notoriously marked for the rice fields, and 2016 the last year of the study period, are analysed thereafter, including ET and WDI patterns.

Figure 4.26 a) Land uses in the Doñana region derived from the Spanish Land Occupation Information System 2013 (SIOSE); b) *ET* mean (mm/year) for the Doñana region over the study period 2003-2016; *ET* (mm/year) and *WDI* values for c) 2005 (dry year, $P=241$ mm), d) 2007 where *ET* reductions were notoriously marked in the rice fields and e) 2016, the last year of the series (676 mm precipitation).

We assessed the standardized anomalies of ET ($STDA_{ET}$) and precipitation ($STDA_P$) for the evaluated land cover classes. The analysis of $STDA_P$ pointed to anomalously dry (2005) and humid (2010) precipitation years, reaching $\Phi_{0,1}(STDA_P)$ values over and below ± 1.64 respectively, which means a probability $P[STDA_P \leq 1.64] = 95\%$ and $P[STDA_P \geq -1.64] = 95\%$ respectively. Generally, $STDA_{ET}$ in the Doñana natural ecosystems were positive (or close to $\overline{ET}$) over 2003 to 2011 (except for year 2005), and negative over 2012 to 2016, following a similar pattern than the standardized anomalies of precipitation $STDA_P$ (Fig. 4.27b). The correlation analysis revealed a significant correspondence between annually aggregated ET versus precipitation P ($R > 0.4$ for the wetland and shrubland), and a strong independent pattern in the irrigated areas (Fig. 4.27a).

Figure 4.27 Annual standardized anomalies and cumulative distribution function $\Phi_{0,1}(STDA_{ET,P})$ showing probability levels of the estimated PT-JPL-thermal ET and precipitation P over 2003-2016 for a) irrigated areas, b) natural ecosystems.

4.3.4.2 Pluri-annual ET periods and trends in the Doñana natural ecosystems

With the focus on the Doñana National Park, where natural ecosystems (wetland, shrubland and coniferous forest) are dependent on precipitation, Fig.4.28 illustrates the presence of two differentiated pluri-annual periods. A more humid period, with positive deviations from $\overline{ET}$ over 2005 to 2011, is followed by a drier period with negative deviations over 2011 to 2016. Particularly for the wetland, ET deviations presented a steeply rising slope from 2005 to 2011 (17% over $\overline{ET}$), more pronounced from 2009 to 2011 (35% over $\overline{ET}$), and a steeply decreasing slope (26% below $\overline{ET}$) from 2011 to 2016. The shrubland followed a similar ET deviations pattern although less pronounced, from positive (25% over $\overline{ET}$ from 2009-2011) to negative slopes (8% below $\overline{ET}$ over 2011-2016). For the coniferous forest, the transition from a positive to negative slope of $CUDM_{ET}$ deviations also occurred in 2011. Regarding precipitation deviations from the mean $CUDM_P$, it was observed similar patterns to natural ecosystems, particularly the wetland. A clear transition from positive to negative deviations occurred in 2010 (ET was 25% higher and 12% lower than $\overline{ET}$ over the periods 2005-2010 and 2010-2016 respectively). As expected from Fig. 4.27a, $CUDM_{ET}$ and $CUDM_P$ were not correlated in the irrigated areas, and the analysis has not been included.

Figure 4.28 Cumulative unitary deviations from the ET mean $CUDM_{ET}$ and cumulative deviations from the P mean $CUDM_P$ in the Doñana natural ecosystems (wetland, shrubland and coniferous forest) over the period 2003-2016.

We analysed annual ET trends in the Doñana region over the study period 2003-2016 by a linear regression model. The R value per pixel for the temporal ET data series showed significant differences amongst land cover classes (Fig. 4.29b). Whereas minimum and negative R values were found in the wetland ($R < -0.5$), maximum and positive values ($R = 0.30$) were located in the rice fields, the central area of the western Natural Park,

and across several areas located in the western boundary of the National and buffered Natural Park (Fig. 4.29b).

Considering the pluri-annual humid (2005-2011) and dry *ET* periods (2011-2016) detected in the *CUDM* analysis for the natural ecosystems (Fig. 4.28), the most pronounced changes on *ET* trends between both periods were found in the Doñana wetland, from positive ($R > 0.3$) over 2005-2011, Fig. 4.29e, to negative ($R < -0.5$) over 2011-2016, Fig. 4.29f. The shrubland and coniferous forest experienced smoother changes on *ET* trends.

Figure 4.29 a) Spanish Land Occupation Information System 2013 (SIOSE); b) *ET* trends in the Doñana region over 2003-2016 expressed as the *R* value of a linear regression model; c) Spanish Land Occupation Information System 2013 (SIOSE), detailed for the Doñana National Park (wetland, shrubland and coniferous forest); *ET* trends in the Doñana National Park d) over the entire period 2003-2016, e) over the more humid period (2005-2011) and f) over the drier period (2011-2016). Red and blue squares account for the lowest and highest *R* values of *ET* trends detected in the region.

A double-mass curve permitted to assess the underlying causes of changes on *ET* trends in the wetland, using as explicative variables precipitation *P*, *NDVI* and *ET_p*. *ET* presented two marked trends: a first period (2005-2011) with an average $\overline{ET} = 775$ mm/year and a second period (2011-2016) with $\overline{ET} = 579$ mm/year, reaching a 25% *ET*

reduction between periods. Precipitation showed a 16% reduction (from $\bar{P}=576$ mm/year to $\bar{P}=481$ mm/year) over the two evaluated periods although ET_p and $NDVI$ did not show however significant trends over the study period (Fig4.30).

Figure 4.30 Double mass curve showing the contribution of P , $NDVI$ and ET_p on ET trend changes in the wetland over the study period 2003-2016.

4.3.5 Discussion

In this study, spatio-temporal daily ET series derived from the PT-JPL-thermal were analysed for the period 2003-2016. We assessed the dynamics and trends of ET in a differentiated land-uses region dominated by combined natural ecosystems and irrigated areas.

4.3.5.1 Spatio-temporal ET dynamics in the Doñana region

Clear differences in daily ET spatio-temporal patterns among land cover classes over the study period 2003-2016 were found in the region, which provides insights on the ET dynamics.

The sensitivity of the PT-JPL-thermal model to precipitation variability is illustrated in Fig.4.25, which shows high correspondence between precipitation amount and ET patterns for natural ecosystems. Annual precipitation and ET standardized anomalies showed high agreement both in humid and dry years for natural ecosystems (Fig. 4.27b), and a strong independent pattern in the irrigated areas (Fig. 4.27a). For our study period we found year 2005, characterized as one of the worst drought episode in the Iberian Peninsula (Garcia-Herrera *et al.*, 2007), anomalously dry ($P [STDA_p \leq 1.64] =$

95%). This drought resulted in an immediate *ET* reduction on natural ecosystems and a more time-lagged effect on irrigated fields. The drought impact on Doñana natural ecosystems was dependent on the vegetation type (Fig. 4.24b and Fig. 4.25). The wetland and shrubland areas were most strongly affected, suffering up to a 55% and a 27% *ET* reduction, while the coniferous forest was not so much affected probably due to its capacity to access shallow phreatic water (Calder *et al.*, 1997). In accordance to these results, Garcia *et al.* (2009) identified the wetland and shrubland as the most sensitive to rainfall variations, whereas the coniferous forest was found to be almost unaffected. The distinct effect of the 2005 drought between irrigated areas and natural ecosystems is spatially illustrated in Fig. 4c. Reddish-orange pixels correspond to those areas with lowest *ET* values (<600 mm/year) and highest water deficits ($WDI < 0.4$), which were more pronounced in the wetland. Greenish pixels represent the highest *ET* values (900 mm/year) and lowest water deficits ($WDI > 0.6$), more pronounced in the rice fields and coniferous forest, which were not affected by the drastic reduction of precipitation.

The effect of the 2005 drought in the irrigated areas could be observed in the period 2006- 2008 (Fig. 4.24a and Fig 4.25), when water in the reservoirs and groundwater reserves were strongly reduced and so that insufficient to meet the irrigation demand (JdA, 2007). The rice fields were particularly affected, with a 50% reduction in the irrigation supply and a 40% in the cultivated area as compared to the period 2002-2005 (JdA, 2007). As shown in Fig. 4.26d, *ET* values within the rice fields in 2007 ranged from 400 to 1000 mm/year showing high spatial variability. Similar patterns were found for *WDI* (values between 0.6 and 0.4). These results are highly significant in an ecological context, since understanding how precipitation anomalies affect vegetation behaviour and their persistence over time and space may contribute to anticipate ecosystems possible responses to climate change (Garcia *et al.*, 2009).

4.3.5.2 Pluri-annual *ET* periods and trends in the Doñana natural ecosystems

The results of the linear regression model over the entire period 2003-2016 identified most negative *ET* trends in the Doñana natural ecosystems, particularly the wetland ($R < -0.43$) (Fig. 4.29b, 4.29d). The largest increase in water use over time ($R > 0.30$) corresponded to: (1) the central area of the western Natural Park, (2) the rice fields, (3) Matalascañas resort and (4) several patches across the North-western area of the Natural Park, where a significant agricultural intensification has happened with strawberries and citrus fruits as main crops (Guardiola-Albert and Jackson, 2011).

Pronounced positive and negative unitary cumulative ET deviations from the mean ($CUDM_{ET}$) were in agreement with precipitation P deviations in the Doñana natural ecosystems (Fig. 4.28), allowing the identification of two pluri-annual periods, a more humid (2005-2011) and drier (2011-2016) in a region where precipitation patterns are predicted to further decrease over time (IPCC, 2015).

In particular, the wetland showed the most significantly consistent agreement between P and ET over the entire study period, indicating the high precipitation-dependence of the wetland (Fig. 4.28). In the last decades, this ecosystem has suffered a transition from mostly alluvial water inputs-dependence to mostly pluvial (Fernández *et al.*, 2010), which results in close to desiccation ponds in years of low precipitation (Díaz-Paniagua and Aragonés, 2015).

For the humid and dry period identified in Fig. 6, the most significant change on ET trends between periods occurred in the wetland, with R values decreasing from positive ($R > 0.3$) over 2005-2011 (Fig. 4.29e) to negative ($R < -0.4$) over 2011-2016 (Fig. 4.29f). This means a 25% ET reduction in the wetland (from $\overline{ET} = 775$ mm/year over 2005-2011 to $\overline{ET} = 579$ over 2011-2016), accounting for approximately 197 m³/ha per year, equivalent to 5,5 hm³/year of ET reduction.

The double-mass curve allowed detecting the underlying explicative variables of changes on ET trends in the wetland (Fig. 4.30). We calculated the trends of atmospheric water demand (ET_p), vegetation greenness ($NDVI$) and water supply (precipitation) for the wetland over the study period. ET_p and $NDVI$ did not show significant trends; precipitation has progressively decreased from 2011 (16% reduction), which may partially explain ET reductions in the wetland, although at lower rates than ET . Land-use changes towards more market-valued uses have lowered the water table of the aquifer to a level that may compromise, also considering expected precipitation deficits (IPCC, 2015), the conservation of the Doñana protected areas. Particularly within the network of piezometers across the aquifer, the level of “Caracoles”, within the wetland, has lowered from 1.4 to 2.6 m in the period of study 2003-2016 (CHG, 2017). Unlicensed greenhouses extend over 6000 ha of the region, extracting groundwater from illegal wells (Guardiola-Albert and Jackson, 2011) at rates of approximately 90 hm³/year on average, a 45% of the aquifer recharge (Custodio *et al.* 2009); this results in reductions on the groundwater contributions to the streams flow rates in the wetland, mostly in summer (Guardiola-Albert and Jackson, 2011). The World Heritage Committee has urged to reverse these over-extraction trends in the area

(UNESCO, 2017) aiming to preserve the integrity of the Doñana associated ecosystems and agricultural sustainable management.

4.3.6 Conclusions

We studied the evapotranspiration responses of natural ecosystems and irrigated lands in the Doñana region of the Mediterranean basin through the PT-JPL-thermal model with a thermal inertial approach to estimate soil moisture over 2003-2016. It resulted a suitable tool for predicting *ET* at regional level, requiring only air temperature and incoming solar radiation apart from standard satellites-products freely available. The daily *ET* spatio-temporal series from the PT-JPL-thermal clearly revealed differentiated and coherent spatio-temporal patterns among the evaluated natural ecosystems and irrigated lands. Increases in water use, shown by positive *ET* temporal trends, were observed for the rice fields and several patches across the north-west area of the National Park, corresponding to areas of intensified agriculture; more pronounced decreases on water consumptions, shown by highly significant *ET* decreasing trends, were found in the Doñana wetlands. Precipitation and *ET* dynamics were highly correlated in the wetlands, although the coniferous forest *ET* showed a very low correlation with *P* due to its capacity to access the water table during drought. The results are consistent with the information obtained by other means and showed the soundness of the model to detect and explain the evolution of the water use and, by extension, to estimate the trends on water uses in future scenarios.

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CHAPTER 5

Main conclusions

5 Conclusions

This work has investigated the potentiality to improve the assessment of the water balance components, especially evapotranspiration ET , in the UNESCO protected semiarid region of Doñana and surrounding irrigated areas. Monitoring ET has significant implications in understanding the hydrological cycle and in the assessment of environmental stresses on both natural ecosystems and agricultural lands. In this study, three different methodologies to track ET , one based on a proposed hydrological model WATEN and the other two based on remote sensing-based combination approaches, were proposed and compared to assess the spatio-temporal dynamics of the ET in the region. The main conclusions derived from this study are presented hereafter.

5.1 Main conclusions

1. The development of an original hydrological model, WATEN, which estimates the ET as a function of the soil moisture content (SMC), allowed quantifying the historical water balance components in the BXII-ID for 10 years of model simulation from 2003 to 2012.
2. WATEN proposes a novel method to organize the model calculations, which proved to reduce the computational requirements and to avoid non-convergences in the calculations, demonstrating the capability of this method for its application to similar cases. This was achieved by introducing an auxiliary variable to resolve the inter-related equations of ET , SMC and drainage D , which permitted to solve the drawbacks derived from the iterative resolution of the three-equation system.
3. In the model calibration, it was proposed to direct the Monte Carlo Simulation method in a similar manner to genetic algorithms. The "Parameters Estimation based on Driven Trials (PEDT)" method proposed herein proved its capability to diminish the computational requirements and resulted in a coherent set of parameters that reached a Nash-Sutcliffe efficiency coefficient $e_2 = 0.90$ between the observed and estimated drainage series.
4. For model calibration data, WATEN proposes an alternative to the traditional streamflow-based data, relying instead on energy consumption at the drainage pumping stations. This aspect is of interest in regions where access to streamflow information is not always available, providing an alternative method that facilitates the monitoring of

the hydrological components of the system, therefore facilitating timely preventive responses particularly in water scarcity areas.

5. MOD16 presented a very pronounced high bias with respect to WATEN-derived *ET* estimates in the study region. The *VPD* alone used by MOD16 for soil evaporation may reflect the surrounding arid conditions but does not consider the availability of water in the soil, particularly important in irrigated areas and in the natural ecosystems within the Doñana region, which rest over the aquifer Almonte-Marismas.

6. The study revealed that MOD16 may be useful to identify those land uses with the lowest and largest *ET* rates, although fail to estimate *ET* at quantitative level. In addition, MOD16 failed to capture the seasonality of the water dynamics for all the evaluated land uses although it captured the inter-annual variability of the water dynamics, indicating its feasibility for inter-annual global studies. It was clearly identified the necessity of alternative RS-based models to more precisely approach the availability of water in the soil thus to better reproduce the seasonality and quantification of the *ET* particularly in semiarid regions.

7. The thermal version of the RS-based Priestley Taylor Jet Propulsion Laboratory model (PT-JPL-thermal), that uses the land surface temperature *LST* as a proxy to track the availability of water in the soil, was computed on a daily basis at the pixel level for 14 years of model simulation from 2003 to 2016, with the novelty of having been regionalized to the semiarid region of Doñana and adjoining irrigated areas, and with a reformulation of the original model with modelled net radiation R_n .

8. The PT-JPL-thermal model reasonably approached the *ET* estimates and dynamics derived from WATEN in the BXII-ID. When extended to the whole Doñana region and surrounding irrigated areas, the model revealed well-differentiated and coherent spatio-temporal patterns in the evaluated land uses (agricultural lands and natural ecosystems) as compared to documented *ET* rates in the region.

9. The model demonstrated capability to differentiate between irrigated areas and natural ecosystems through the identification of either the immediate or time-lagged effect of droughts respectively.

10. Significant differences were also found within the natural ecosystems themselves, where the model permitted to discretize the differentiated effect of drought and the different responses to precipitation *P* dynamics. Throughout the years, the *ET*

was found highly correlated with P in the wetlands, and to a much lower extent in the shrublands, forests and croplands. This suggests that the wetlands may be most susceptible to overall drying, though the whole region is susceptible. The model proved to provide essential information in the context of climatic changes, significantly important to identify those ecosystems more capable or unable to adapt to water availability changes given the right information at the right time, mainly under scenarios of droughts.

11. The analysis of the ET trends allowed to distinguish hot-spots or areas where the water use for natural ecosystems was declining or sites where the water use was significantly increasing throughout the study period. These results may help to inform water management decisions and consequences when balancing regional demands for food production and ecological sustainability.

12. Although the hydrological WATEN has proven simplicity and reasonably well-adjusted model results in the application to this study, it operates as a semi-distributed model in which it is not possible to find spatial differences within an area previously classified. Instead, this study has shown that satellite-based data may significantly enhance the spatial distribution of ET in a simple manner which circumvents the over-parameterization of the system which may have possibly derived from transforming WATEN into a distributed model.

13. In this study, the PT-JPL-thermal has demonstrated to be a suitable and simple tool requiring only air temperature and incoming solar radiation apart from standard satellite-products freely available, especially interesting in areas with scarce availability of data. In addition, this study proves that the use of the thermal inertia concept as a proxy indicator to the water availability in the soil, together with the re-formulation of the outgoing longwave radiation, makes it possible to reasonably reproduce the dynamics of the ET in water-limited regions, where other RS-based models failed to success, particularly in the Doñana region and surroundings.

5.2 Main highlights

- WATEN allowed estimating the hydrological components of the system, particularly *ET* as a function of the soil moisture content, by proposing an alternative calibration methodology based on the energy consumption data.
- MOD16 failed to capture the quantification and the seasonality of the water dynamics in the region, with the only reliable results in terms of inter-annual *ET* variability patterns, indicating its feasibility for inter-annual global studies.
- The PT-JPL-thermal model, reformulated with modelled net radiation made it possible to reasonably reproduce the dynamics of the *ET* in a water-limited region where other RS-based had failed.
- The use of the thermal inertia concept instead of the *VPD* alone as a proxy to the availability of water in the soil makes it possible to reasonably reproduce the dynamics of the *ET* in water-limited regions.
- The regionalization of the PT-JPL-thermal in this study has demonstrated the model to be a suitable tool requiring only climatic data and satellite-data freely available to estimate *ET* in semiarid regions with scarce availability of data.

5.3 Future work

- Challenges facing water managers in arid and semiarid regions include salinity increases and pollution from various sources. The assessment of the historical evolution of drainage discharge to the Guadalquivir River obtained through the original model WATEN may represent a first step in the quantification of the discharge of nitrates and salts from the District to the River in an area where many of the surrounding croplands, rice fields and wetlands area designated as nitrate vulnerable zones under the European Commission nitrates Directive.
- Despite the significant advances on *ET* based science modelling, there are still outstanding knowledge gaps to estimate *ET* more precisely. Although MOD16 uses the Penman-Monteith PM approach, theoretically more accurate than Priestley-Taylor used in the PT-JPL-thermal model, the proxy used by MO16 for water availability has been proved to fail particularly in semiarid regions. Further research on the Penman-Monteith approach, introducing the thermal inertia approach used by the PT-JPL-thermal, could lead to more accurate estimations of *ET* in semiarid regions, when the availability of data may allow its application.

- At regional level, the incorporation of more reliable spatio-temporal RS-based *ET* estimations in commonly used hydrological models where *ET* is estimated based on meteorological data, e.g. the SIMPA model (Estrela Monreal and Quintas Ripoll, 1996; Ruiz-García, 1999) in Spain would allow improving the study of water resources in terms of *ET* regionalization, leading to a more precise calibration of other less-precise variables involved in the water balance at national level.

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APPENDIXES

Appendix I. Downloading MODIS products for the implementation of the PT-JPL-thermal (as in March 2018)

1. Visualize the specific “granule” and lat/long

MODIS Overview: https://lpdaac.usgs.gov/dataset_discovery/modis

- Go to MODIS Sinusoidal Tiling System.
- Visualize the grid or granule. For Doñana: MODIS h/v: h17v05.
- USGS Global Visualization Viewer GloVis: <https://glovis.usgs.gov/>.
- Visualize lat/long : about 37/-6 for a central point in Doñana.

2. Visualize MODIS land products

MODIS data products table:

https://lpdaac.usgs.gov/dataset_discovery/modis/modis_products_table

Site to visualize MODIS products to download. Products are divided between Terra (day products), Aqua (night products), and combined-products.

3. Choose and download MODIS products

EarthData Search: <https://search.earthdata.nasa.gov/search>

- Insert the code of the product chosen in the MODIS product table.
- Insert the range of dates.
- Select the area: ->point-> go to specific lat/long in the map.
- Select the data to download-> view/download data links.
- A list with all the selected images for the selected granule appears.
- A text file is generated-> save it in a folder.

4. Save MODIS images into our computer

- **The required images are still on the “cloud”**, but the URL address to access them is in the text file generated. Thus, we need a programme to download these images into our computer.
- **We install Daac2Disk** https://lpdaac.usgs.gov/data_access/daac2disk
Once Daac2Disk is installed->use the command prompt. Note: the text file should be saved as a .txt file into the same directory that the Daac2Disk.exe file.
- **Using the command prompt to download images with Daac2Disk**
The command prompt is a command line interpreter application available in most Windows operating systems. Command Prompt is a Windows program that emulates many of the command line abilities available in MS-DOS but it is not actually MS-DOS.

Instructions to the command prompt

Cd c:\MODISdlw (where the text file generated is saved)

Daac2Disk_win.exe --inputfile nameofthetxtfile.txt --output C:\MODISdl

Note: it is very important to add .txt at the end of the url text file

- **The images will be automatically downloaded** in the same folder where the text file is located (e.g. c:\MODISdl)

Appendix II. Frequency of the MODIS products required for the implementation of the PT-JPL-thermal model

- **Vegetation Index**

MOD13A2. VI Terra. First date: 2012_001

MYD13A2. VI Aqua. First date: 2012_009

MODIS captures an image of the “granule” on a daily basis. Only the “best” image of a 16-days period is downloadable for the VI product (e.g. NDVI). Terra 16-days period begins January 1st every year. Aqua 16-days period starts January 9th every year. Thus, there are two different 16-composite VI products: one product derived from Terra: MOD13A2 and one derived from Aqua: MYD13A2. Thus, there is a VI image every 8 days, one from the Terra 16-days composite and one from the Aqua 16-days composite. Note: MYD13A2 presents an overlap in January for adjusting the days of the year.

- **$LAI f_{APAR}$**

MOD15A2. $LAI f_{APAR}$ Terra

MYD15A2. $LAI f_{APAR}$ Aqua

MODIS captures an image of the “granule” on a daily basis. Only the “best” image of an 8-days period is downloadable for the $LAI f_{APAR}$ product. Both Terra and Aqua start the composite period every January 1st.

- **Albedo**

MCD43B3 Albedo

The MODIS Albedo product presents the same frequency characteristics as the VI (see above). However, MODIS Albedo is a combined product, i.e. both 16-days period “best” image from both Aqua and Terra is presented in one single product.

- **Surface temperature**

MOD11A1 Temperature Terra

[MYD11A1 Temperature Aqua](#)

MODIS captures an image of the “granule” every day. Daily images are downloadable.

Appendix III. Programming the PT-JPL-thermal model for regionalization on Matlab

% This script permits to calculate evapotranspiration at spatio temporal scales based on land surface energy fluxes.

% 1 CALCULATION OF THE BIOPHYSICAL CONSTRAINTS **% 2 CALCULATION OF NET RADIATION**

% Read input textfiles

```
[a1]=textread('F:\MODIS\MOD13A2_NDVI_T\URL\NDVI_T\NDVI_T_corre.txt','%s',
'whitespace','\n');
[a2]=textread('F:\MODIS\MOD15A2_LAI\APAR\URL\APAR\APAR_corre.txt','%s',
'whitespace','\n');
[a3]=textread('F:\MODIS\MYD11A1_LST_A\URL\Emis31_Emis32\Emis31_A_corre.t
xt','%s','whitespace','\n');
[a4]=textread('F:\MODIS\MYD11A1_LST_A\URL\Emis31_Emis32\Emis32_A_corre.t
xt','%s','whitespace','\n');
[a5]=textread('F:\MODIS\MOD11A1_LST_T\URL\Emis31_Emis32\Emis31_T_corre.tx
t','%s','whitespace','\n');
[a6]=textread('F:\MODIS\MOD11A1_LST_T\URL\Emis31_Emis32\Emis32_T_corre.t
xt','%s','whitespace','\n');
[a7]=textread('F:\MODIS\MYD11A1_LST_A\URL\Tday\Tday_A_corre.txt','%s','white
space','\n');
[a8]=textread('F:\MODIS\MOD11A1_LST_T\URL\Tday\Tday_T_corre.txt','%s','white
space','\n');
[a9]=textread('F:\MODIS\MYD11A1_LST_A\URL\Tday_Tnight_timepass\Tday_time
pass_A_corre.txt','%s','whitespace','\n');
[a10]=textread('F:\MODIS\MOD11A1_LST_T\URL\Tday_Tnight_timepass\Tday_time
pass_T_corre.txt','%s','whitespace','\n');
[a11]=textread('F:\MODIS\MCD43B3_Albedo\URL\Albedo_BSA_WSA\Albedo_BSA
_corre.txt','%s','whitespace','\n');
[a12]=textread('F:\MODIS\MCD43B3_Albedo\URL\Albedo_BSA_WSA\Albedo_WS
A_corre.txt','%s','whitespace','\n');
```

% Read output textfiles

```
[b32]= textread('F:\Modelfruit2017\fc_fg_Terra\fc.txt','%s','whitespace','\n');
[b33]= textread('F:\Modelfruit2017\fc_fg_Terra\fg.txt','%s','whitespace','\n');
[b34]= textread('F:\Modelfruit2017\fm_fm.txt','%s','whitespace','\n');
[b35]= textread('F:\Modelfruit2017\ft\ft.txt','%s','whitespace','\n');

[b37]= textread('F:\Modelfruit2017\Rlw\Rlw_in.txt','%s','whitespace','\n');
[b38]= textread('F:\Modelfruit2017\Rlw\Rlw_out.txt','%s','whitespace','\n');
[b39]= textread('F:\Modelfruit2017\Rsw\Rsw_daily.txt','%s','whitespace','\n');
[b40]= textread('F:\Modelfruit2017\Rsw\Rsw_inst.txt','%s','whitespace','\n');
[b41]= textread('F:\Modelfruit2017\Rn\Rn_inst.txt','%s','whitespace','\n');
[b42]= textread('F:\Modelfruit2017\Rn\Rn_daily.txt','%s','whitespace','\n');
```

% Load fAPARmax.mat for fM calculations

```
cd('F:\MODIS\MOD15A2_LAI\APAR\URL\APAR')
load fAPARmax.mat
fAPARmax=fAPARmax(523:644,300:400);
```

% Read input excel sheet climaticdata for 2003-2016

```
cd('F:\Model\ClimaticNOAA')
[numbers string]=xlsread('climaticdata2003_2016_fruits.xlsx','2013_2016');
Tmean=numbers(3:end,11);
Tmax=numbers(3:end,5);
Tmin=numbers(3:end,8);
Rad=numbers(3:end,17);
```

% Read input excel sheet NOAA trise and tsunset for 2003-2016

```
[numbers string]=xlsread('NOAA_2003_2012_corr.xlsx','trise_sunset_N_2013_2016');
trise=numbers(3:end,3);
tsunset=numbers(3:end,5);
N=numbers(3:end,6);
```

```
for i=1:length(a1);
```

```
    i
```

% Open the files for binary read (r) access (fopen)

```
    cd('F:\MODIS\MOD13A2_NDVI_T\URL\NDVI_T');
        cell_name1 = a1(i,1);
        string_name1 = char(cell_name1);
        fileid1(i) = fopen(string_name1,'r');
    cd('F:\MODIS\MOD15A2_LAI\APAR\URL\APAR');
        cell_name2 = a2(i,1);
        string_name2 = char(cell_name2);
        fileid2(i) = fopen(string_name2,'r');
    cd('F:\MODIS\MYD11A1_LST_A\URL\Emis31_Emis32');
        cell_name3 = a3(i,1);
        string_name3 = char(cell_name3);
        fileid3(i) = fopen(string_name3,'r');
        cell_name4 = a4(i,1);
        string_name4 = char(cell_name4);
        fileid4(i) = fopen(string_name4,'r');
    cd('F:\MODIS\MOD11A1_LST_T\URL\Emis31_Emis32');
        cell_name5 = a5(i,1);
        string_name5 = char(cell_name5);
        fileid5(i) = fopen(string_name5,'r');
        cell_name6 = a6(i,1);
        string_name6 = char(cell_name6);
        fileid6(i) = fopen(string_name6,'r');
    cd('F:\MODIS\MYD11A1_LST_A\URL\Tday');
        cell_name7 = a7(i,1);
        string_name7 = char(cell_name7);
        fileid7(i) = fopen(string_name7,'r');
    cd('F:\MODIS\MOD11A1_LST_T\URL\Tday');
        cell_name8 = a8(i,1);
```

```

    string_name8 = char(cell_name8);
    fileid8(i) = fopen(string_name8,'r');
cd('F:\MODIS\MYD11A1_LST_A\URL\Tday_Tnight_timepass');
    cell_name9 = a9(i,1);
    string_name9 = char(cell_name9);
    fileid9(i) = fopen(string_name9,'r');
cd('F:\MODIS\MOD11A1_LST_T\URL\Tday_Tnight_timepass');
    cell_name10 = a10(i,1);
    string_name10 = char(cell_name10);
    fileid10(i) = fopen(string_name10,'r');
cd('F:\MODIS\MCD43B3_Albedo\URL\Albedo_BSA_WSA');
    cell_name11 = a11(i,1);
    string_name11 = char(cell_name11);
    fileid11(i) = fopen(string_name11,'r');
    cell_name12 = a12(i,1);
    string_name12 = char(cell_name12);
    fileid12(i) = fopen(string_name12,'r');

% Open the files for binary writing (w) access (fopen)
cd('F:\Modelfruit2017\fc_fg_Terra')
    cell_name32 = b32(i,1);
    fileid33(i) = fopen(string_name33,'w');
cd('F:\Modelfruit2017\fm')
    cell_name34 = b34(i,1);
    string_name34 = char(cell_name34);
    fileid34(i) = fopen(string_name34,'w');
cd('F:\Modelfruit2017\ft')
    cell_name35 = b35(i,1);
    string_name35 = char(cell_name35);
    fileid35(i) = fopen(string_name35,'w');
cd('F:\Modelfruit2017\RIw')
    cell_name37 = b37(i,1);
    string_name37 = char(cell_name37);
    fileid37(i) = fopen(string_name37,'w');
    cell_name38 = b38(i,1);
    string_name38 = char(cell_name38);
    fileid38(i) = fopen(string_name38,'w');
cd('F:\Modelfruit2017\Rsw')
    cell_name39 = b39(i,1);
    string_name39 = char(cell_name39);
    fileid39(i) = fopen(string_name39,'w');
    cell_name40 = b40(i,1);
    string_name40 = char(cell_name40);
    fileid40(i) = fopen(string_name40,'w');
cd('F:\Modelfruit2017\Rn')
    cell_name41 = b41(i,1);
    string_name41 = char(cell_name41);
    fileid41(i) = fopen(string_name41,'w');
    cell_name42 = b42(i,1);
    string_name42 = char(cell_name42);

```

```

fileid42 (i) = fopen(string_name42 , 'w');

% Read the input binary files
cd ('F:\MODIS\MOD13A2_NDVI_T\URL\NDVI_T')
NDVI_T=fread(fileid1(i),[1200 1200],'int16');
cd ('F:\MODIS\MOD15A2_LAI\APAR\URL\APAR')
fAPAR=fread(fileid2(i),[1200 1200],'uint8');
cd ('F:\MODIS\MYD11A1_LST_A\URL\Emis31_Emis32')
Emis31_A=fread(fileid3(i),[1200 1200],'uint8');
Emis32_A=fread(fileid4(i),[1200 1200],'uint8');
cd ('F:\MODIS\MOD11A1_LST_T\URL\Emis31_Emis32')
Emis31_T=fread(fileid5(i),[1200 1200],'uint8');
Emis32_T=fread(fileid6(i),[1200 1200],'uint8');
cd ('F:\MODIS\MYD11A1_LST_A\URL\Tday')
Tday_A=fread(fileid7(i),[1200 1200],'uint16');
cd ('F:\MODIS\MOD11A1_LST_T\URL\Tday')
Tday_T=fread(fileid8(i),[1200 1200],'uint16');
cd ('F:\MODIS\MYD11A1_LST_A\URL\Tday_Tnight_timepass')
Tday_A_timepass=fread(fileid9(i),[1200 1200],'uint8');
cd ('F:\MODIS\MOD11A1_LST_T\URL\Tday_Tnight_timepass')
Tday_T_timepass=fread(fileid10(i),[1200 1200],'uint8');
cd ('F:\MODIS\MCD43B3_Albedo\URL\Albedo_BSA_WSA')
Albedo_BSA=fread(fileid11(i),[1200 1200],'int16');
Albedo_WSA=fread(fileid12(i),[1200 1200],'int16');

% Convert to double precision
NDVI_T=double(NDVI_T);
fAPAR=double(fAPAR);
Emis31_A=double(Emis31_A);
Emis32_A=double(Emis32_A);
Emis31_T=double(Emis31_T);
Emis32_T=double(Emis32_T);
Tday_A=double(Tday_A);
Tday_T=double(Tday_T);
Tday_A_timepass=double(Tday_A_timepass);
Tday_T_timepass=double(Tday_T_timepass);
Albedo_BSA=double(Albedo_BSA);
Albedo_WSA=double(Albedo_WSA);

% Valid ranges
NDVI_T(NDVI_T<-2000)= NaN;
NDVI_T(NDVI_T>10000)= NaN;
fAPAR(fAPAR<0)=NaN;
fAPAR(fAPAR>100)=NaN;
Emis31_A(Emis31_A<1)= NaN;
Emis31_A(Emis31_A>255)= NaN;
Emis32_A(Emis32_A<1)= NaN;
Emis32_A(Emis32_A>255)= NaN;
Emis31_T(Emis31_T<1)= NaN;
Emis31_T(Emis31_T>255)= NaN;

```



```

Emis32_T(Emis32_T<1)= NaN;
Emis32_T(Emis32_T>255)= NaN;
Tday_A(Tday_A<7500)= NaN;
Tday_A(Tday_A>65535)= NaN;
Tday_T(Tday_T<7500)= NaN;
Tday_T(Tday_T>65535)= NaN;
Tday_A_timepass(Tday_A_timepass<0)= NaN;
Tday_A_timepass(Tday_A_timepass>240)= NaN;
Tday_T_timepass(Tday_T_timepass<0)= NaN;
Tday_T_timepass(Tday_T_timepass>240)= NaN;
Albedo_BSA(Albedo_BSA<0)= NaN;
Albedo_BSA(Albedo_BSA>32766)= NaN;
Albedo_WSA(Albedo_WSA<0)= NaN;
Albedo_WSA(Albedo_WSA>32766)= NaN;

```

% Boundary to the region

```

NDVI_T=NDVI_T(523:644,300:400);
fAPAR=fAPAR(523:644,300:400);
Emis31_A=Emis31_A(523:644,300:400);
Emis32_A=Emis32_A(523:644,300:400);
Emis31_T=Emis31_T(523:644,300:400);
Emis32_T=Emis32_T(523:644,300:400);
Tday_A=Tday_A(523:644,300:400);
Tday_T=Tday_T(523:644,300:400);
Tday_A_timepass=Tday_A_timepass(523:644,300:400);
Tday_T_timepass=Tday_T_timepass(523:644,300:400);
Albedo_BSA=Albedo_BSA(523:644,300:400);
Albedo_WSA=Albedo_WSA(523:644,300:400);

```

% Scaling following MODIS product table

https://lpdaac.usgs.gov/dataset_discovery/modis/modis_products_table

```

NDVI_T=NDVI_T*0.0001;
fAPAR=fAPAR*0.01;
Emis31_A=Emis31_A*0.002+0.49;
Emis32_A=Emis32_A*0.002+0.49;
Emis31_T=Emis31_T*0.002+0.49;
Emis32_T=Emis32_T*0.002+0.49;
Tday_A= Tday_A*0.02;
Tday_T= Tday_T*0.02;
Tday_A_timepass=Tday_A_timepass*0.1;
Tday_T_timepass=Tday_T_timepass*0.1;
Albedo_BSA=Albedo_BSA*0.0010;
Albedo_WSA=Albedo_WSA*0.0010;

```

% Valid range after double and scaling

```

NDVI_T(NDVI_T<0)= NaN;
NDVI_T(NDVI_T>1)= NaN;
%fAPAR_T(fAPAR_T<0)=NaN;
%fAPAR_T(fAPAR_T>1)=NaN;

```

% 1 LOOP CALCULATION OF THE BIOPHYSICAL CONSTRAINTS**% 1.1 GREEN CANOPY FRACTION***% Defining parameters for fIPAR*

m2=1.0;

c2=-0.05

fIPAR_T=m2*NDVI_T+c2;

fc=fIPAR_T;

fc(fc<0)= 0;

fc(fc>1)= 1;

fg= fAPAR./fc;

fg(fg<0)= 0;

fg(fg>1)= 1;

% 1.2 PLANT MOISTURE CONSTRAINT

fM=fAPAR./fAPARmax ;

fM(fM<0)= 0;

fM(fM>1)= 1;

% 1.3 PLANT TEMPERATURE CONSTRAINT

Tmean_day=ones(122,101)*Tmean(i);

fT=1.1814.*(1./(1+exp(0.3.*(-25-10-Tmean_day)))).*1./

(1+exp(0.2.*(25-10-Tmean_day))) ; *% Note: we have changed the (+)Tmean in the first part of the Eq.by(-) Tmean, see Garcia (2013)*

fT(fT<0)=0;

fT(fT>1)=1;

% Write binary data to file

cd('F:\Modelfruit2017\fc_fg_Terra')

status1 = fwrite(fileid32(i),fc,'double');

status2 = fwrite(fileid33(i),fg,'double');

cd('F:\Modelfruit2017\fm');

status3 = fwrite(fileid34(i),fM,'double');

cd('F:\Modelfruit2017\ft');

status4 = fwrite(fileid35(i),fT,'double');

% 2 LOOP CALCULATION OF NET RADIATION (DAILY)**% 2.1 LONGWAVE RADIATION****% Incoming longwave radiation***% Scaling Tair2012 at MODIS pass time (based on Parton and Logan(1981)**% Creating a Tday_time MODIS pass matrix**% Take an average tday_time pass value of the area,ignoring NaN values*

Modis_passtime = nanmean(nanmean(Tday_A_timepass));

Timepass=isnan(Modis_passtime); *%If Modis_passtime is NaN, Timepass acquires value 1 (true)*

```

if Timepass==1;%If Timepass did result NaN, we use Terra Timepass values
instead:
Modis_passtime=nanmean(nanmean(Tday_T_timepass));
end

```

```

% Applying Parton and Logan (1981) for calculating Tair at MODIS pass time
c1=-0.17; % c= lag of the minimum temperature from the time of sunrise,
(parameter following table 1, p.210)
d1=1.86; % d= d refers to a in Parton &Logan, (parameter following table 1,
p.210)
BB=12-(N(i)/2)+c1;
BBD=Modis_passtime-BB; % BBD, number of hours after the minimum T
occurs until sunset
Tair_MODIS_passtime=(Tmax(i)-Tmin(i))*
sin((pi*BBD)/(N(i)+2*d1))+Tmin(i);

```

```

% Calculating incoming longwave radiation
Stef=5.67e-008;
C=0.261;
d=7.77e-004;
Rlw_in=Stef*((Tair_MODIS_passtime+273.15)^4)*(1-(C*exp(-
d*(Tair_MODIS_passtime^2))));

```

% Outgoing longwave radiation

```

% Emissivity(average matrix Emis31-Emis32)
zA= cat(3, Emis31_A,Emis32_A);
zT =cat(3, Emis31_T,Emis32_T);
EmisA=mean(zA,3);
EmisT=mean(zT,3);

```

```

% Calculating outgoing longwave radiation
indices= isnan (EmisA); % find those elements (pixels) where Emis_A is NaN
EmisA (indices)=EmisT (indices); % replace those NaN elements in Emis_A by
Tday_T elements
Emis=EmisA;
indices= isnan (Tday_A); % find those elements (pixels) where Tday_A is NaN
Tday_A (indices)= Tday_T (indices); %replace those NaN elements in Tday_A
by Tday_T elements
Tday=Tday_A;
Rlw_out=-Stef*Emis.*(Tday.^4);

```

% Total longwave radiation

```

Rlw=Rlw_in+Rlw_out;

```

% 2.2 SHORTWAVE RADIATION**% Incoming shortwave radiation (MJ/m2/day)**

```
Rsw_in_MJ=Rad(i); % from MJ/m2/day to W/m2 (1J=1W.s)
Rsw_in=Rsw_in_MJ*(1000000/(3600*24)); %(W/m2)
```

% Total shortwave radiation

```
Rsw_daily=(ones(122,101)*Rsw_in).*(1-(0.8*Albedo_BSA+
0.2*Albedo_WSA)); % (w/m2)
```

% Scaling shortwave radiation from daily to instantaneous

```
t=Modis_passtime-trise(i);
J=2/(pi*(sin(pi*t/N(i))));
Rsw_inst= Rsw_daily/J*(24/(N(i)));
```

% 2.3a TOTAL NET RADIATION (INSTANTANEOUS)

```
Rn_inst=Rlw+Rsw_inst;
```

% 2.3b TOTAL NET RADIATION (FROM INSTANTANEOUS TO DAILY)

```
Rn_daily=Rn_inst*J*N(i)/24;
```

% Write binary data to file

```
cd('F:\Modelfruit2017\Rlw')
status8 = fwrite (fileid37(i),Rlw_in,'double');
status9 = fwrite(fileid38(i),Rlw_out,'double');
cd('F:\Modelfruit2017\Rsw\')
status10 = fwrite(fileid39(i),Rsw_daily,'double');
status11 = fwrite (fileid40(i),Rsw_inst,'double');
cd('F:\Modelfruit2017\Rn\')
status12 = fwrite (fileid41(i),Rn_inst,'double');
status13 = fwrite (fileid42(i),Rn_daily,'double');
```

% Close all open files

```
status = fclose('all');
fileid = fclose('all');
```

```
end
```

% 3 CALCULATION OF THE NET RADIATION PARTITION**% 4 CALCULATION OF POTENTIAL EVAPOTRANSPIRATION****% 5 CALCULATION OF ACTUAL CANOPY TRANSPIRATION LEC****% Read input textfiles**

```
[a13]=textread('F:\MODIS\MOD15A2_LAI\APAR\URL\LAI\LAI_corre.txt','%s','white
space','\n');
```

```
[a14]= textread('F:\Modelfruit2017\Rn\Rn_daily.txt','%s','whitespace','\n');
[a15]= textread('F:\Modelfruit2017\fc_fg_Terra\fc.txt','%s','whitespace','\n');
[a16]= textread('F:\Modelfruit2017\fc_fg_Terra\fg.txt','%s','whitespace','\n');
[a17]= textread('F:\Modelfruit2017\ft\ft.txt','%s','whitespace','\n');
[a18]= textread('F:\Modelfruit2017\fm\fm.txt','%s','whitespace','\n');
```

% Read output textfiles

```
[b44]= textread('F:\Modelfruit2017\Rn\Rns.txt','%s','whitespace','\n');
[b45]= textread('F:\Modelfruit2017\Rn\Rnc.txt','%s','whitespace','\n');
[b46]= textread('F:\Modelfruit2017\ETp\Etpc.txt','%s','whitespace','\n');
[b47]= textread('F:\Modelfruit2017\ETp\Etps.txt','%s','whitespace','\n');
[b48]= textread('F:\Modelfruit2017\ETp\Etp.txt','%s','whitespace','\n');
[b49]= textread('F:\Modelfruit2017\AE\AE.txt','%s','whitespace','\n');
[b50]= textread('F:\Modelfruit2017\LEc\LEc.txt','%s','whitespace','\n');
```

% Read input excel sheet climaticdata for 2003-2016

```
cd('F:\Model\ClimaticNOAA')
[numbers string]=xlsread('climaticdata2003_2016_fruits.xlsx','2013_2016');
% Select Tmean column
Tmean=numbers(3:end,11);
```

```
for i=1:length(a13);
    i
    % Open the files for binary read (r) access (fopen)
    cd('F:\MODIS\MOD15A2_LAI\APAR\URL\LAI')
    cell_name13 = a13(i,1);
    string_name13 = char(cell_name13);
    fileid13(i) = fopen(string_name13,'r');
    cd('F:\Modelfruit2017\Rn\')
    cell_name14 = a14(i,1);
    string_name14 = char(cell_name14);
    fileid14(i) = fopen(string_name14,'r');
    cd('F:\Modelfruit2017\fc_fg_Terra\')
    cell_name15 = a15(i,1);
    string_name15 = char(cell_name15);
    fileid15(i) = fopen(string_name15,'r');
    cd('F:\Modelfruit2017\fc_fg_Terra')
    cell_name16 = a16(i,1);
    string_name16 = char(cell_name16);
    fileid16(i) = fopen(string_name16,'r');
    cd('F:\Modelfruit2017\ft')
    cell_name17 = a17(i,1);
    string_name17 = char(cell_name17);
    fileid17(i) = fopen(string_name17,'r');
    cd('F:\Modelfruit2017\fm')
    cell_name18 = a18(i,1);
    string_name18 = char(cell_name18);
    fileid18(i) = fopen(string_name18,'r');
```

% Open the files for binary writing (w) access (fopen)

```
cd('F:\Modelfruit2017\Rn')
    cell_name44 = b44(i,1);
    string_name44 = char(cell_name44);
    fileid44(i) = fopen(string_name44,'w');
    cell_name45 = b45(i,1);
    string_name45 = char(cell_name45);
    fileid45(i) = fopen(string_name45,'w');
```

```
cd('F:\Modelfruit2017\ETp')
    cell_name46 = b46(i,1);
    string_name46 = char(cell_name46);
    fileid46(i) = fopen(string_name46,'w');
    cell_name47 = b47(i,1);
    string_name47 = char(cell_name47);
    fileid47(i) = fopen(string_name47,'w');
    cell_name48 = b48(i,1);
    string_name48 = char(cell_name48);
    fileid48(i) = fopen(string_name48,'w');
```

```
cd('F:\Modelfruit2017\AE')
    cell_name49 = b49(i,1);
    string_name49 = char(cell_name49);
    fileid49(i) = fopen(string_name49,'w');
```

```
cd('F:\Modelfruit2017\LEc')
    cell_name50 = b50(i,1);
    string_name50 = char(cell_name50);
    fileid50(i) = fopen(string_name50,'w');
```

% Read the input binary files

```
cd('F:\MODIS\MOD15A2_LAI\APAR\URL\LAI')
    LAI = fread(fileid13(i),[1200 1200],'uint8');
cd('F:\Modelfruit2017\Rn')
    Rn_daily= fread(fileid14(i),[122 101],'double');
cd('F:\Modelfruit2017\fc_fg_Terra')
    fc = fread(fileid15(i),[122 101],'double');
cd('F:\Modelfruit2017\fc_fg_Terra')
    fg = fread(fileid16(i),[122 101],'double');
cd('F:\Modelfruit2017\ft')
    ft = fread(fileid17(i),[122 101],'double');
cd('F:\Modelfruit2017\fm')
    fm = fread(fileid18(i),[122 101],'double');
```

% Convert to double precision

```
LAI=double(LAI);
```

% Valid ranges

```
LAI(LAI<0)=NaN;
LAI(LAI>100)=NaN;
```

% Boundary to the region

LAI=LAI(523:644,300:400);

% Scaling following MODIS product table

LAI=LAI*0.1;

% 3 LOOP CALCULATION OF THE NET RADIATION PARTITION**% 3.1 NET RADIATION TO THE SOIL**

% Defining parameters

kRn=0.6; *% García et al(2013)based on Impens&Lemeur (1969)*

% Rns is calculated as in García et al (2013), following Beer (1852) according to Fisher et al. (2008)

Rns= Rn_daily.*exp(-kRn*LAI); *% (Wm-2)*

% 3.2 NET RADIATION TO THE CANOPY

Rnc=Rn_daily-Rns;

% 4 LOOP CALCULATION OF POTENTIAL EVAPOTRANSPIRATION**% 4.1 CANOPY POTENTIAL EVAPOTRANSPIRATION**

% Coefficient of Priestley-Taylor (1972)

alfaPT=1.26; *% used in García et al (2013) and Fisher et al (2008).*

% Psychrometric constant (psi)

% Atmospheric pressure at elevation z (P)

elev=25; *%(m) Altitud of Lebrija I (IFAPA)*

P=101.3*(((293-0.0065*elev)/293)^5.26); *% (kPa)*

% Latent Heat of Vaporization (lambda)

lambda=2454-2.4*(Tmean(i)-20); *% (kJ/kg)*

% Specific heat of moist air (cp)

cp=1013; *%(kJ kg-1 °C-1)*

% Ratio molecular weight of water vapor/dry air

epsi=0.622;

% Calculatino of psychrometric constant (psi)

psi=(cp*P)/(epsi*lambda); *% (Pa)*

% Saturation vapor pressure(es)

es=10*(0.061121*2.718281828.^(17.502*Tmean(i)./(240.97+Tmean(i))))*(1.0007+(3.46*10.^(-8)*100));

% Slope vapor pressure curve (s)

s=(lambda*18*1000*es)/(8.3144*(Tmean(i)+273)^2);

% Calculation of canopy potential evapotranspiration Etpc following Priestley Taylor

Etpc=alfaPT*(s/(s+psi))*Rnc; *%(Wm-2)*

% 4.2 SOIL POTENTIAL EVAPOTRANSPIRATION

% Soil heat flux (G) "Soil heat flux (G) should be included in available soil energy (Rns-G), but where G is unavailable, Rns may be used alone" Fisher (2008) based on Kustas et al (1993). Norman et al (1995) assumes $G=0.35 \cdot R_{nsoil}$

G=0;

Etps=alfaPT*(s/(s+psi))*(Rns-G); % (Wm-2)

% 4.3 TOTAL POTENTIAL EVAPOTRANSPIRATION

Etp=Etpc+Etps; % (Wm-2)

AE=Rn_daily-G; % (Wm-2)

% 5 LOOP CALCULATION OF ACTUAL CANOPY TRANSPIRATION LEc

LEc=fg.*ft.*fM.*Etpc; % (Wm-2)

% Write binary data to file

status11 = fwrite (fileid44(i),Rns,'double');

status12 = fwrite (fileid45(i),Rnc,'double');

status13= fwrite (fileid46(i),Etpc,'double');

status14 = fwrite (fileid47(i),Etps,'double');

status15 = fwrite (fileid48(i),Etp,'double');

status16 = fwrite (fileid49(i),AE,'double');

status17 = fwrite (fileid50(i),LEc,'double');

% Close all open files

status = fclose('all');

fileid = fclose('all');

end

clear all

% 6 CALCULATION OF ATI**% Read input textfiles**

[a19]=textread('F:\MODIS\MCD43B3_Albedo\URL\Albedo_BSA_WSA\Albedo_BSA_corre.txt','%s','whitespace','\n'); % lists input files albedo BSA

[a20]=textread('F:\MODIS\MCD43B3_Albedo\URL\Albedo_BSA_WSA\Albedo_WSA_corre.txt','%s','whitespace','\n'); % lists input files albedo WSA

[a21]=textread('F:\MODIS\MOD11A2_LST_T_8days\URL\Tday\Tday_T_corre.txt','%s','whitespace','\n'); % lists input files Tday_T

[a22]=textread('F:\MODIS\MYD11A2_LST_A_8days\URL\Tday\Tday_A_corre.txt','%s','whitespace','\n'); % lists input files Tday_A

[a23]=textread('F:\MODIS\MOD11A2_LST_T_8days\URL\Tnight\Tnight_T_corre.txt','%s','whitespace','\n'); % lists input files Tnight_T

[a24]=textread('F:\MODIS\MYD11A2_LST_A_8days\URL\Tnight\Tnight_A_corre.txt','%s','whitespace','\n'); % lists input files Tnight_A

% Read output textfiles

```
[b51] = textread('F:\Modelfruit2017\ATI\ATI.txt','%s','whitespace','\n'); % lists output files ATI
```

% Read input excel sheet climaticdata for 2003-2016

```
cd('F:\Model\ClimaticNOAA')
[numbers string]=xlsread('climaticdata2003_2016_fruits.xlsx','2013_2016');
% Select Tmean column
Tmean=numbers(3:end,11);
```

% Read the latitude textfile for ATI calculation (derived from programme eos2dump)

```
cd('F:\Modelfruit2017\ATI')
lat1D = load(['lat_MOD11A1.A2012001.h17v05.005.2012016233639.output']);
% Reshape lat data into an array format
lat = reshape(lat1D, 1200, 1200);
clear lat1D;
% Change lat data to radians(http://www.gabrielortiz.com/index.asp?Info=058a)
lat=(lat*pi)/180;
% Transpose array
lat = lat';
% Boundary to region
lat= lat(523:644,300:400);
```

```
for i=1:length(a19);
```

```
    i
```

% Open the files for binary read (r) access (fopen)

```
    cd('F:\MODIS\MCD43B3_Albedo\URL\Albedo_BSA_WSA')
    cell_name19 = a19(i,1);
    string_name19 = char(cell_name19);
    fileid19(i) = fopen(string_name19,'r');
    cell_name20 = a20(i,1);
    string_name20 = char(cell_name20);
    fileid20(i) = fopen(string_name20,'r');
    cd('F:\MODIS\MOD11A2_LST_T_8days\URL\Tday')
    cell_name21 = a21(i,1);
    string_name21 = char(cell_name21);
    fileid21(i) = fopen(string_name21,'r');
    cd('F:\MODIS\MYD11A2_LST_A_8days\URL\Tday')
    cell_name22 = a22(i,1);
    string_name22 = char(cell_name22);
    fileid22(i) = fopen(string_name22,'r');
    cd('F:\MODIS\MOD11A2_LST_T_8days\URL\Tnight')
    cell_name23 = a23(i,1);
    string_name23 = char(cell_name23);
    fileid23(i) = fopen(string_name23,'r');
    cd('F:\MODIS\MYD11A2_LST_A_8days\URL\Tnight')
    cell_name24 = a24(i,1);
    string_name24 = char(cell_name24);
    fileid24(i) = fopen(string_name24,'r');
```

```

% Open the files for binary writing (w) access (fopen)
cd('F:\Modelfruit2017\ATI')
cell_name51 = b51(i,1);
string_name51 = char(cell_name51);
fileid51(i) = fopen(string_name51,'w');

% Read the input binary files
cd('F:\MODIS\MCD43B3_Albedo\URL\Albedo_BSA_WSA')
Albedo_BSA=fread(fileid19(i),[1200 1200],'int16');
Albedo_WSA=fread(fileid20(i),[1200 1200],'int16');
cd('F:\MODIS\MOD11A2_LST_T_8days\URL\Tday')
Tday_T=fread(fileid21(i),[1200 1200],'uint16');
cd('F:\MODIS\MYD11A2_LST_A_8days\URL\Tday')
Tday_A=fread(fileid22(i),[1200 1200],'uint16');
cd('F:\MODIS\MOD11A2_LST_T_8days\URL\Tnight')
Tnight_T=fread(fileid23(i),[1200 1200],'uint16');
cd('F:\MODIS\MYD11A2_LST_A_8days\URL\Tnight')
Tnight_A=fread(fileid24(i),[1200 1200],'uint16');

% Convert to double precision
Albedo_BSA=double(Albedo_BSA);
Albedo_WSA=double(Albedo_WSA);
Tday_T=double(Tday_T);
Tday_A=double(Tday_A);
Tnight_T=double(Tnight_T);
Tnight_A=double(Tnight_A);

% Valid ranges
Albedo_BSA(Albedo_BSA<0)=NaN;
Albedo_BSA(Albedo_BSA>32766)=NaN;
Albedo_WSA(Albedo_WSA<0)=NaN;
Albedo_WSA(Albedo_WSA>32766)=NaN;
Tday_T(Tday_T<7500)=NaN;
Tday_T(Tday_T>65535)=NaN;
Tday_A(Tday_A<7500)=NaN;
Tday_A(Tday_A>65535)=NaN;
Tnight_T(Tnight_T<7500)=NaN;
Tnight_T(Tnight_T>65535)=NaN;
Tnight_A(Tnight_A<7500)=NaN;
Tnight_A(Tnight_A>65535)=NaN;

% Boundary to the region
Albedo_BSA=Albedo_BSA(523:644,300:400);
Albedo_WSA=Albedo_WSA(523:644,300:400);
Tday_T=Tday_T(523:644,300:400);
Tday_A=Tday_A(523:644,300:400);
Tnight_T=Tnight_T(523:644,300:400);
Tnight_A=Tnight_A(523:644,300:400);

```

% Scaling following MODIS product table

```

Albedo_BSA=Albedo_BSA*0.0010;
Albedo_WSA=Albedo_WSA*0.0010;
Tday_T=Tday_T*0.02;
Tday_A=Tday_A*0.02;
Tnight_T=Tnight_T*0.02;
Tnight_A= Tnight_A*0.02;

```

% 6 LOOP CALCULATION OF ATI

```

% Calculation of maximum temperature per day

```

```

% Replace Tday_A NaN values by Tday_T values when NaN

```

```

indices= isnan (Tday_A); % find those elements (pixels) where Tday_A is
NaN

```

```

Tday_A (indices)=Tday_T (indices); % replace those NaN elements in
Tday_A by Tday_T values.

```

```

% Choose maximum T value between Tday_A and Tday_T

```

```

indices = Tday_T > Tday_A; Tday_T > Tday_A conducts element by
element comparisons, with elements set to logical 1 where the
relationship is true and elements set to logical 0 where it is not

```

```

% In Tday_A replace those elements found greater in Tday_T

```

```

Tday_A(indices) = Tday_T(indices);

```

```

% Calculation of minimum temperature per day

```

```

% Replace Tnight_A NaN values by Tnight_T values when NaN

```

```

indices= isnan (Tnight_A); % find those elements (pixels) where night_A
is NaN

```

```

Tnight_A (indices)=Tnight_T (indices); % replace those NaN elements in
Tnight_A by Tnight_T values.

```

```

% Choose minimum T value between Tnight_A and Tnight_T

```

```

indices = Tnight_T < Tnight_A;
Tnight_A(indices) = Tnight_T(indices);

```

```

% Day angle and solar declination based on:

```

```

http://naturalfrequency.com/Tregenza\_Sharpley/Daylight\_Algorithms/algorithm\_1\_1\_1.htm

```

```

day_angle=2*pi*(i-1)/366;
solar_declination=0.006918-0.399912*cos(day_angle)+0.070257*
sin(day_angle)-0.006758*cos(2*day_angle)+0.000907*sin(2*day_angle)
-0.002697*cos(3*day_angle)+0.001480*sin(3*day_angle);
solar_decl=solar_declination;

```

```

% Solar correction factor

```

```

solar_correction_factor=sin(lat)*sin(solar_decl).*(1-(((tan(lat)).^2)*
((tan(solar_decl))^2)))+(cos(lat)*cos(solar_decl).*acos((-tan(lat))*
tan(solar_decl)));
scf=solar_correction_factor;

```

```

% Calculation of ATI based on Verstraeten et al (2006)

```

```

ATI=scf.*((ones(122,101)-(0.8*Albedo_BSA+0.2*Albedo_WSA))./
(Tday_A-Tnight_A)); % as in García et al (2013)

```

```

        ATI(ATI<0)=0;
        ATI(ATI>0.1125)=0.1125;

% Write binary data to file
        cd ('F:\Modelfruit2017\ATI')
        status18 = fwrite(fileid51(i),ATI,'double');

% Close all open files
        fileid = fclose('all');
        status = fclose('all');
end

```

% 7 CALCULATION OF fSM-ATI

% Calculating ATImin and ATImax

% Create artificial ATImin and ATImax arrays for comparison with the first ATI, when day i=1

```

        ATImax = ones(122,101).*-100000;
        ATImin = ones(122,101).*100000;

```

% Read ATI textfile as input (binary files generated in the previous loop)

```

        [a70] = textread('F:\Modelfruit2017\ATI\ATI.txt','%s','whitespace','\n');

```

% Loop for ATImax and ATImin calculations

```

for i=1:length(a70);
    i
    % Open the binary files for read access (fopen)
        cd('F:\Modelfruit2017\ATI\')
        cell_name70 = a70(i,1);
        string_name70 = char(cell_name70);
        fileid70(i) = fopen(string_name70,'r');

% Read the input binary files
        ATI=fread(fileid70(i),[122 101],'double');

% Obtaining ATImax
        indices = ATI > ATImax;
        ATImax(indices) = ATI(indices);

% Obtaining ATImin
        indices = ATI < ATImin;
        ATImin(indices) = ATI(indices);

% Close all open files
        status = fclose('all');
end

```

% Save ATImax and ATImin

```
cd('F:\Modelfruit2017\ATI')
save ATImax ATImax; % Save a matlab file with the variable ATImax.
save ATImin ATImin; % Save a matlab file with the variable ATImin.
```

% Read input textfiles

```
[a25] = textread('F:\Modelfruit2017\ATI\ATI.txt','%s','whitespace','\n');
```

% Read output textfiles

```
[b52]= textread('F:\Modelfruit2017\ATI\FSM_ATI.txt','%s','whitespace','\n');
```

% Loop for fSM_ATI calculations

```
for i=1:length(a25);
    i
    % Open the files for binary read access (fopen)
    cd('F:\Modelfruit2017\ATI\')
    cell_name25 = a25(i,1);
    string_name25 = char(cell_name25);
    fileid25(i) = fopen(string_name25,'r');

    % Open the files for binary writing (w) access (fopen)
    cell_name52 = b52(i,1);
    string_name52 = char(cell_name52);
    fileid52(i) = fopen(string_name52,'w');

    % Read the input binary files
    ATI=fread(fileid25(i),[122 101],'double');

    % 7 LOOP CALCULATION OF fSM_ATI
    fSM_ATI=(ATI-ATImin)./(ATImax-ATImin);

    % Write binary data to file
    Status19 = fwrite(fileid52(i),fSM_ATI,'double');

    % Close all open files
    status=fclose('all')
end
```

% 8 CALCULATION OF ACTUAL SOIL EVAPORATION LEs**% Read input textfiles**

```
[a26] = textread('F:\Modelfruit2017\ETp\Etps.txt','%s','whitespace','\n');
[a27] = textread('F:\Modelfruit2017\ATI\FSM_ATI.txt','%s','whitespace','\n');
```

% Read output textfiles

```
[b53]= textread('F:\Modelfruit2017\LEs\LEs.txt','%s','whitespace','\n');
```

```

for i=1:length(a26);
    i
    % Open the files for binary read access (fopen)
    cd('F:\Modelfruit2017\ETp\')
    cell_name26 = a26(i,1);
    string_name26 = char(cell_name26);
    fileid26(i) = fopen(string_name26,'r');
    cd('F:\Modelfruit2017\ATI\')
    cell_name27 = a27(i,1);
    string_name27 = char(cell_name27);
    fileid27(i) = fopen(string_name27,'r');

    % Open the files for binary writing (w) access (fopen)
    cd('F:\Modelfruit2017\LEs\')
    cell_name53= b53(i,1);
    string_name53 = char(cell_name53);
    fileid53(i) = fopen(string_name53,'w');

    % Read the input binary files
    Etps=fread(fileid26(i),[122 101],'double');
    fSM_ATI=fread(fileid27(i),[122 101],'double');

    % 8 LOOP CALCULATION OF ACTUAL SOIL EVAPORATION LEs
    LEs= fSM_ATI.*Etps;%(Wm-2)

    % Write binary data to file
    status20 = fwrite(fileid53(i),LEs,'double');

    % Close all open files
    status=fclose('all')
    fileid = fclose('all');

end

% 9 CALCULATION OF ACTUAL EVAPOTRANSPIRATION LE

% Read input textfiles
[a28] = textread('F:\Modelfruit2017\LEc\LEc.txt','%s','whitespace','\n');
[a29] = textread('F:\Modelfruit2017\LEs\LEs.txt','%s','whitespace','\n');

% Read output textfiles
[b54]= textread('F:\Modelfruit2017\LE\LE.txt','%s','whitespace','\n');
[b57]= textread('F:\Modelfruit2017\ET\ET.txt','%s','whitespace','\n');

% Read input excel sheet climaticdata for 2003-2016
cd('F:\Model\ClimaticNOAA')
[numbers string]=xlsread('climaticdata2003_2016_fruits.xlsx','2013_2016');
% Select Tmean column
Tmean=numbers(3:end,11);

```

```

for i=1:length(a28);
    i
    % Open the files for binary read access (fopen)
    cd('F:\Modelfruit2017\LEc\')
    cell_name28 = a28(i,1);
    string_name28 = char(cell_name28);
    fileid28(i) = fopen(string_name28,'r');

    cd('F:\Modelfruit2017\LEs\')
    cell_name29 = a29(i,1);
    string_name29 = char(cell_name29);
    fileid29(i) = fopen(string_name29,'r');

    % Open the files for binary writing (w) access (fopen)
    cd('F:\Modelfruit2017\LE\')
    cell_name54= b54(i,1);
    string_name54 = char(cell_name54);
    fileid54(i) = fopen(string_name54,'w');
    cd('F:\Modelfruit2017\ET\')
    cell_name57= b57(i,1);
    string_name57 = char(cell_name57);
    fileid57(i) = fopen(string_name57,'w');

    % Read the input binary files
    LEc=fread(fileid28(i),[122 101],'double');
    LEs=fread(fileid29(i),[122 101],'double');

    % 9 LOOP CALCULATION OF ACTUAL EVAPOTRANSPIRATION LE
    LE=LEs+LEc;%(Wm-2)

    % Conversion of LE into ET
    % Calculate lambda
    lambda=(2454-2.4*(Tmean(i)-20))/1000;%(MJ/kg)
    ET=(LE/lambda)*0.0864; %(mm/day)

    % Write binary data to file
    status21 = fwrite(fileid54(i),LE,'double');
    status22 = fwrite(fileid57(i),ET,'double');

    % Close all open files
    status=fclose('all');
    fileid = fclose('all');

end

% 10 CALCULATION OF EF AND WDI

% Read input textfiles
[a28] = textread('F:\Modelfruit2017\AE\AE.txt','%s','whitespace','\n');

```

```
[a29] = textread('F:\Modelfruit2017\Etp\Etp.txt','%s','whitespace','\n');
[a30] = textread('F:\Modelfruit2017\LE\LE.txt','%s','whitespace','\n');
```

% Read output textfiles

```
[b55]= textread('F:\Modelfruit2017\EF\EF.txt','%s','whitespace','\n');
[b56]= textread('F:\Modelfruit2017\WDI\WDI.txt','%s','whitespace','\n');
```

```
for i=1:length(a29);
    i
    % Open the files for binary read access (fopen)
    cd('F:\Modelfruit2017\AE')
    cell_name28 = a28(i,1);
    string_name28 = char(cell_name28);
    fileid28(i) = fopen(string_name28,'r');
    cd('F:\Modelfruit2017\Etp')
    cell_name29 = a29(i,1);
    string_name29 = char(cell_name29);
    fileid29(i) = fopen(string_name29,'r');
    cd('F:\Modelfruit2017\LE')
    cell_name30 = a30(i,1);
    string_name30 = char(cell_name30);
    fileid30(i) = fopen(string_name30,'r');

    % Open the files for binary writing (w) access (fopen)
    cd ('F:\Modelfruit2017\EF')
    cell_name55= b55(i,1);
    string_name55 = char(cell_name55);
    fileid55(i) = fopen(string_name55,'w');

    cd ('F:\Modelfruit2017\WDI')
    cell_name56= b56(i,1);
    string_name56 = char(cell_name56);
    fileid56(i) = fopen(string_name56,'w');

    % Read the input binary files
    AE=fread(fileid28(i),[122 101],'double');
    Etp=fread(fileid29(i),[122 101],'double');
    LE=fread(fileid30(i),[122 101],'double');

    % 10 LOOP CALCULATION OF EF AND WDI
    EF=LE./AE; WDI=LE./Etp;

    % Write binary data to file
    status23 = fwrite (fileid55(i),EF,'double');
    status24 = fwrite (fileid56(i),WDI,'double');

    % Close all open files
    status = fclose('all');
    fileid = fclose('all');
end
```