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Magnitude and variability of
terrestrial evaporation from satellites
and climate reanalyses

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Grootte-orde en variabiliteit van evapotranspiratie afgeleid uit satellietwaarnemingen en klimaatreanalyse data

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Cover

The cover picture is designed by Anabelle Michiels and shows an artistic impression of the annual terrestrial evaporation estimated using the Global Land Evaporation Amsterdam Model (GLEAM).

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Working towards a doctoral degree – and doing scientific research in general – is (and should) always be a team effort: you need supervisors¹ that guide you through this journey, and advice you at the right moment; you need peers to discuss your findings or methods, and help you to see things differently; you need colleagues that apparently do way more fancy stuff than you do, and push you to explore new horizons; you need friends that are a bit skeptical about your job, thereby encouraging you to proof them wrong; and you need family that listens to you, and puts a smile upon your face, every day again. Luckily enough, I could count on an exceptionally large team. Although I cannot thank each of you in person here, I think everybody that deserves a thank you probably knows by now.

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¹Yes, supervisorS. Some PhD candidates only have one supervisor and most (I guess) have two supervisors. However, I have been classified as one of these special cases that needs a lot of supervision, and got assigned three supervisors.

²Honestly, I know for a fact that Hans had more important things to do that day. On top of that, I already met him before.

study how soil moisture can be estimated from satellite data. On a more serious note, Hans is a fantastic scientist, and he taught me all the technical details of soil moisture retrieval from satellites and – more importantly – how these retrievals can be made useful by ingesting them into hydrological models. Hans, I want to thank you for all our technical discussions we had over the years, for all your critical (but useful) comments on my articles, for involving me in your own research, for all the fun we had while having a beer, and for teaching me how to get the most out of scientific conferences; i.e. discussing science during dinner with a good beer.

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³I am not sure if Diego meant this, or if he just wanted to challenge me at that time, but I believe the exact number he mentioned was 20 publications.

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List of Acronyms

AIRS	Atmospheric InfraRed Sounder
ALEXI	Atmosphere–Land EXchange Inverse
AMM	Atlantic Meridional Mode
AMO	Atlantic Multidecadal Oscillation
AMSR-E	Advanced Microwave Scanning Radiometer for Earth
ARM	Atmospheric Radiation Measurement network
BELSPO	BELgian Science Policy Office
CATDS	Centre Aval de Traitement des Données SMOS
CCI	Climate Change Initiative
CDF	Cumulative Distribution Function
CERES	Clouds and Earth’s Radiant Energy System
CESAR	Cabauw Experimental Site for Atmospheric Research
CI	Climate Index
CONUS	CONtinental United States
COSMO	CONsortium for Small-scale MOdeling
COSMO-REA6	COSMO-REAnalysis version 6
EA	East Atlantic pattern
EASE	Equal Area Scalable Earth
EAWR	East Atlantic West Russia pattern
ECMWF	European Centre for Medium-range Weather Forecasts
ECV	Essential Climate Variable
ENSO	El Niño Southern Oscillation
EPNP	East Pacific North Pacific pattern
ERA	ECMWF’s ReAnalysis
ESA	European Space Agency
EUMETSAT	EUropean organisation for METeorological SATellites
GCOS	Global Climate Observing System
GEWEX	Global Energy and Water-cycle EXperiment
GLDAS	Global Land Data Assimilation System
GLEAM	Global Land Evaporation Amsterdam Model

GLEAM+ERA-I	GLEAM forced with ERA-I
GLEAM+ERA5	GLEAM forced with ERA5
GLEAM-HR	GLEAM High Resolution
GRACE	Gravity Recovery And Climate Experiment
GRDC	Global Runoff Data Centre
H-TESEL	Hydrology Tiled ECMWF Scheme for Surface Exchanges over Land
ICOS	Integrated Carbon Observation System
IFS	Integrated Forecast System
IGBP	International Geosphere–Biosphere Programme
IOD	Indian Ocean Dipole
IPCC	Intergovernmental Panel on Climate Change
ISBA	Interactions between Soil, Biosphere, and Atmosphere
ISMN	International Soil Moisture Network
JMA	Japanese Meteorological Agency
JRA-55	Japanese 55-year ReAnalysis
KNMI	<i>Koninklijk Nederlands Meteorologisch Instituut</i> Royal Meteorological Institute of The Netherlands
LASSO	Least Absolute Shrinkage and Selection Operator
LPRM	Land Parameter Retrieval Model
LSA-SAF	Land Surface Analysis Satellite Application Facility
LST	Land Surface Temperature
MAD	Mean Absolute Difference
MD	Mean Difference
MERRA	Modern Era Retrospective-Analysis for research
MODIS	MODerate-resolution Imaging Spectroradiometer
MSG	Meteosat Second Generation
MSWEP	Multi-Source Weighted-Ensemble Precipitation
MTE	Multi-Tree Ensemble
NAM	Northern Annular Mode
NAO	North Atlantic Oscillation
NASA	National Aeronautics and Space Administration
NEON	National Ecological Observatory Network
NEWS	NASA Energy and Water cycle Study
NOAA	National Oceanic and Atmospheric Administration
NSIDC	National Snow and Ice Data Center
OL	Open Loop
PDO	Pacific Decadal Oscillation
PEA	Polar EurAsia pattern
PML	Penman Monteith Leuning
PNA	Pacific-North American pattern
PT-JPL	Priestley Taylor Jet Propulsion Laboratory algorithm

RMSD	Root Mean Squared Difference
RSS	Residual Sum of Squares
SAM	Southern Annular Mode
SEB	Surface Energy Balance
SEBAL	Surface Energy Balance Algorithm for Land
SEBS	Surface Energy Balance System
SEVIRI	Spinning Enhanced Visible and InfraRed Imager
SIF	Solar-Induced Fluorescence
SMMR	Scanning Multichannel Microwave Radiometer
SMOS	Soil Moisture and Ocean Salinity
SSM/I	Special Sensor Microwave/Imager
TCA	Triple Collocation Analysis
TERENO	TERrestrial EnviroNmental Observatories
TIR	Thermal InfraRed
TNA	Tropical Northern Atlantic dipole
TRMM	Tropical Rainfall Measuring Mission
TSA	Tropical Southern Atlantic dipole
TSS	Total Sum of Squares
UNFCCC	United Nations Framework Convention on Climate Change
ubMAD	unbiased MAD
ubRMSD	unbiased RMSD
VOD	Vegetation Optical Depth
VPD	Vapour Pressure Deficit
WACMOS	WATER Cycle Multimission Observation Strategy
WATCH	WATER and global CHange project
WCRP	World Climate Research Programme
WMO	World Meteorological Organisation
WP	West Pacific pattern

List of Symbols

α	Priestley and Taylor coefficient (-)
β	vector of regression coefficients (-)
β_b	Bowen ratio (-)
γ	quality factor in Newtonian Nudging (-)
Δ	slope of saturated water vapour-temperature curve ($\text{Pa}\cdot\text{K}^{-1}$)
ϵ	terrestrial energy storage ($\text{J}\cdot\text{m}^{-2}$)
ϑ	vegetation optical depth (-)
κ	empirical parameter in Equation 2.3
λ	latent heat of vaporisation ($\text{J}\cdot\text{kg}^{-1}$)
$\lambda\rho E$	surface latent heat flux ($\text{W}\cdot\text{m}^{-2}$)
ρ	density of water ($\text{kg}\cdot\text{m}^{-3}$)
σ_{mod}	standard deviation of model errors of soil moisture ($\text{m}^3\cdot\text{m}^{-3}$)
σ_{obs}	standard deviation of observation errors of soil moisture ($\text{m}^3\cdot\text{m}^{-3}$)
ψ	psychometric constant ($\text{Pa}\cdot\text{K}^{-1}$)
ω	regularisation parameter (-)
Ω^n	Gaussian kernel with one-sided width n (-)
CO_2	carbon dioxide (-)
E	terrestrial evaporation ($\text{m}\cdot\text{s}^{-1}$)
E_i	interception loss ($\text{m}\cdot\text{s}^{-1}$)
E_p	potential evaporation ($\text{m}\cdot\text{s}^{-1}$)
F_f	fast draining flux of water ($\text{m}\cdot\text{s}^{-1}$)
F_s	slow draining flux of water ($\text{m}\cdot\text{s}^{-1}$)
G	ground heat flux ($\text{W}\cdot\text{m}^{-2}$)
H	surface sensible heat flux ($\text{W}\cdot\text{m}^{-2}$)
K	nudging factor in Newtonian Nudging (-)
n	number of samples in data set (-)
p	number of features in data set (-)
P	precipitation ($\text{m}\cdot\text{s}^{-1}$)
q_{25}	25% quantile of a data set
q_{75}	75% quantile of a data set

Q	river discharge ($\text{m}\cdot\text{s}^{-1}$)
R	Pearson correlation coefficient (-)
R^2	explained variance of a model (-)
R_n	surface net radiation ($\text{W}\cdot\text{m}^{-2}$)
s	volume of terrestrial water storage per unit area (m)
S	evaporative stress factor (-)
$T_{2\text{m}}$	2-meter air temperature ($^{\circ}\text{C}$)
w	soil moisture ($\text{m}^3\cdot\text{m}^{-3}$)
w_c	critical soil moisture ($\text{m}^3\cdot\text{m}^{-3}$)
w_p	soil porosity ($\text{m}^3\cdot\text{m}^{-3}$)
w_r	residual soil moisture ($\text{m}^3\cdot\text{m}^{-3}$)
w_{wp}	wilting point ($\text{m}^3\cdot\text{m}^{-3}$)
W	interpolation weight in Newtonian Nudging (-)
x	independent variable in regression model (-)
y	dependent variable in regression model (-)
$\cdot_i$	i^{th} variable (-)
$\cdot_{\text{an}}$	statistic calculated at anomalies (-)
$\cdot_{\text{max}}$	maximum of a variable (-)
$\cdot_{\text{min}}$	minimum of a variable (-)
$\cdot_{\text{san}}$	statistic calculated at standardised anomalies (-)
$\cdot_t$	variable at time step t (-)
$\cdot^{(l)}$	variable at layer l of GLEAM (-)
$\cdot^o$	observation of a variable (-)
$\cdot^{(w)}$	variable at the wettest soil layer in GLEAM (-)
$\cdot^+$	a posteriori model state (-)
$\cdot^-$	a priori model state (-)
$\hat{\cdot}$	model estimate of a variable (-)
$\langle\cdot\rangle$	anomaly of a variable (-)

Summary

Terrestrial evaporation (often referred to as *evapotranspiration*) is the total volume of water that is returned from the land surface into the atmosphere and is – after precipitation – the second largest flux in the terrestrial hydrological cycle. The flux consists of the vaporisation of water through vegetation (transpiration), directly from the soil (bare soil evaporation), from wet canopies (interception loss), and from snow-covered surfaces (sublimation). Transpiration is generally the dominant component and is closely related to the process of carbon assimilation in plants known as photosynthesis. Hence, terrestrial evaporation acts as a link between the terrestrial water and carbon cycles. In addition, given the high energy requirements to evaporate water, terrestrial evaporation also controls the partitioning of energy at the ecosystem level and the cycling of energy in the atmosphere, thereby affecting for instance air temperature, humidity, cloud formation, and the occurrence of precipitation. Next to being a crucial variable to understand our Earth system, the flux is essentially a net loss of water from the land surface and is therefore also key for society. Accurate information on terrestrial evaporation is necessary to properly manage our water resources, thereby securing the availability of drinking water, and the production of energy and food. Altogether, terrestrial evaporation data at different spatio-temporal scales is thus valuable for different disciplines ranging from climatology, ecology, and hydrology, to agricultural planning, operational drought monitoring, and water resources management.

Despite the importance of terrestrial evaporation, the flux is still one of the most uncertain and elusive variables of the hydrological cycle, especially at the global scale, which hampers the assessment of its global-scale magnitude, temporal variability, and response to variations in climate. However, also at local and regional scales, accurate and timely information on terrestrial evaporation with the required spatio-temporal detail is often lacking, thereby impeding for instance water resources management, agricultural planning, and hydrological forecasting. The main reason for this lack of information is that, still today, it is particularly difficult to monitor terrestrial evaporation.

While in situ measurements provide relatively accurate information, they are only representative for a small region surrounding the measuring site. In contrast, satellite-based observations yield data over large areas, but terrestrial evaporation cannot be directly “seen” from satellite platforms and mathematical algorithms are a necessary tool to derive estimates of terrestrial evaporation from satellite-based variables closely related to the process of evaporation; hence, introducing substantial errors in the final estimates.

Given the difficulties to obtain accurate data on terrestrial evaporation, the overarching objective of this dissertation is to support different disciplines and research fields in need of these data at different spatio-temporal scales by providing high-quality, satellite-based, and observational data sets of terrestrial evaporation. In addition, it is also aimed to explore the assets of these data sets in two case studies within the field of hydro-climatology and climate reanalysis. More specifically, the three key objectives of this dissertation are formulated as:

1. To support global hydrological, atmospheric, and climate studies by deriving a global data set of terrestrial evaporation from satellite data at coarse spatial resolution (i.e. ± 25 km).
2. To aid local water resources management and agricultural planning by deriving a pilot data set of terrestrial evaporation for The Netherlands, Flanders, and the west of Germany from satellite data at high spatial resolution (i.e. 100 m).
3. To reveal the potential of the global data set derived in this dissertation for benchmarking climate reanalyses and to advance our understanding of the global-scale variability of terrestrial evaporation.

To meet these objectives, advancing the Global Land Evaporation Amsterdam Model (GLEAM) – a process-based model dedicated to the estimation of terrestrial evaporation and its components from satellite-based data at the global scale – is the first point of focus in this dissertation (Chapters 2 and 3). Therefore, Chapter 2 explores the potential of satellite-based surface soil moisture to improve continental-scale estimates of terrestrial evaporation via data assimilation, a technique merging observations and model estimates of the same variable based on their relative errors. In a study over continental Australia, the impact of different options in the data assimilation system are explored, and their added value is evaluated by using in situ validation data. In Chapter 3, the data assimilation system and various other model components in GLEAM are further improved to better represent the land surface control on the terrestrial evaporation process. Chapter 3 also presents results from a comprehensive global-scale validation of terrestrial evaporation and root-zone soil moisture, derived using this new version of GLEAM.

Chapter 4 of this dissertation assesses the potential of GLEAM to be applied at high resolution and to derive root-zone soil moisture and terrestrial evaporation at scales useful for local water resources management and agricultural planning. In this chapter, a pilot data set of terrestrial evaporation at 100 m spatial resolution for The Netherlands, Flanders, and the west of Germany is presented and validated using in situ measurements of surface soil moisture and terrestrial evaporation.

The final objective of this dissertation is to explore the assets of GLEAM in two case studies (Chapters 5 and 6). In Chapter 5, GLEAM is used as a tool to evaluate the quality of different reanalysis data sets. In particular, GLEAM is used (1) to evaluate the skill of the land surface scheme in the reanalysis framework and (2) to assess the quality of the atmospheric drivers of terrestrial evaporation in the reanalysis data set. These analyses provide useful insights in the quality of these data sets for global hydrological and climate studies. Chapter 6 investigates the multi-decadal, global-scale variability of terrestrial evaporation – derived using GLEAM – and its link to internal climate variability, which is driven by the most prominent climate modes such as the El Niño Southern Oscillation (ENSO).

Finally, in Chapter 7, a summary of the most important conclusions of this dissertation is given, together with the main limitations, and a path forward to further advance GLEAM and to steer research on the monitoring of terrestrial evaporation is presented.

Samenvatting

Terrestrische verdamping (vaak wordt de term *evapotranspiratie* of gewoonweg verdamping gebruikt) is het totaal volume water dat vanop het landoppervlak terug naar de atmosfeer wordt getransporteerd en is – na neerslag – de grootste flux van water in de landcomponent van de hydrologische cyclus. De flux bestaat uit de verdamping van water via huidmondjes van planten (transpiratie), de directe verdamping van water uit de bodem, de verdamping van water gecapteerd op vegetatie (interceptieverlies), en de verdamping van sneeuw of ijs (sublimatie). Transpiratie is typisch de dominante component en is sterk gerelateerd aan het proces van koolstoffixatie in planten, beter gekend als fotosynthese. Verdamping vormt dus de link tussen de water- en koolstofcyclus op het land. Gezien de grote hoeveelheden energie die nodig zijn om water te verdampen, is verdamping verder ook een proces dat de verdeling van de beschikbare energie op het niveau van ecosystemen controleert en de energiecycclus in de atmosfeer beïnvloedt. Tegelijkertijd heeft verdamping dus een effect op ondermeer de luchttemperatuur, luchtvochtigheid, wolkenvorming, en neerslag. Naast het feit dat verdamping een essentiële variabele is om het Aardse systeem te begrijpen, kan de flux ook gezien worden als een nettoverlies van water vanop het landoppervlak; het is dus eveneens een belangrijk proces voor de mens. Accurate informatie over verdamping is nodig om onze watervoorraden op een gedegen manier te beheren en zo de beschikbaarheid van drinkwater en de productie van energie en voedsel veilig te stellen. Samengevat zijn gegevens over verdamping op verschillende ruimte-tijd schalen van belang voor verschillende disciplines gaande van klimatologie, ecologie, en hydrologie tot irrigatieplanning, operationele droogte monitoring, en waterbeheer.

Ondanks het belang van verdamping, is de flux nog steeds één van de meest onzekere variabelen binnen de hydrologische cyclus, en dit vooral op globale schaal, wat de evaluatie van het totale volume verdamping op wereldniveau bemoeilijkt, alsook de analyse van de temporele variabiliteit en de inschatting van de impact van variaties in het klimaat op de flux. Echter, ook op lokaal en regionaal niveau ontbreekt vaak nauwkeurige en tijdige informatie

van verdamping met de vereiste ruimtelijke en temporele details, waardoor bijvoorbeeld operationeel waterbeheer, irrigatieplanning, en hydrologische voorspellingen worden belemmerd. De belangrijkste reden voor dit gebrek aan data is dat het nog steeds – tot op vandaag – bijzonder moeilijk is om verdamping accuraat te meten of in te schatten. Enerzijds bieden metingen in het veld relatief nauwkeurige informatie. Echter, deze zijn slechts representatief voor een klein gebied rondom de meetlocatie. Anderzijds leveren satellietwaarnemingen gegevens van verschillende hydrologische variabelen over grote gebieden. Echter, verdamping kan niet direct worden “gezien” vanop satellieten, en wiskundige algoritmes zijn noodzakelijk om schattingen van verdamping af te leiden uit satellietwaarnemingen van variabelen die nauw verband houden met het proces van verdamping, en die wel kunnen geobserveerd worden. Als gevolg kunnen wezenlijke fouten in de schattingen van verdamping worden geïntroduceerd door het gebruik van wiskundige modellen in combinatie met onzekere observaties van verschillende gerelateerde variabelen. Gegeven de moeilijkheden om accurate verdampingsdata te verkrijgen, is het overkoepelende doel van dit proefschrift om verschillende disciplines en onderzoeksvelden te ondersteunen die nauwkeurige verdampingsgegevens nodig hebben op verschillende ruimtetijdschalen door nauwkeurige, satelliet-gebaseerde datasets van verdamping af te leiden. Bovendien zullen ook de voordelen van deze datasets onderzocht worden in twee *case studies* in het gebied van hydro-klimatologie en *climate reanalysis*. Meer specifiek worden de drie objectieven van dit proefschrift als volgt geformuleerd:

1. Het ondersteunen van globale hydrologische, atmosferische, en klimatologische studies door het afleiden van een globale dataset van verdamping uit satellietwaarnemingen op grove ruimtelijke schaal (i.e. ± 25 km).
2. Het ondersteunen van waterbeheer en irrigatieplanning door het afleiden van een pilootdataset van verdamping voor Nederland, Vlaanderen, en het westen van Duitsland uit satellietwaarnemingen op fijne ruimtelijke schaal (i.e. 100 m).
3. Het aantonen van het potentieel van de globale dataset, afgeleid in dit proefschrift, voor het evalueren van *climate reanalysis* datasets en om onze kennis over de variabiliteit van verdamping op globale schaal uit te breiden.

Teneinde deze doelstellingen te bereiken, is het eerste punt van focus in dit proefschrift het verder ontwikkelen van het *Global Land Evaporation Amsterdam Model* (GLEAM), een proces-gebaseerd model dat ontworpen werd om verdamping en zijn afzonderlijke componenten uit satellietwaarnemingen te schatten op de globale schaal (Hoofdstukken 2 en 3). Hoofdstuk 2 onderzoekt het potentieel van satellietwaarnemingen van bodemvocht om schattingen van

verdamping op continentale schaal te verbeteren via data assimilatie, een techniek waarbij observaties en modelschattingen van een variabele worden gecombineerd tot een betere schatting, op basis van hun relatieve onzekerheden. De studie wordt uitgevoerd over Australië en de impact van verschillende opties in het data-assimilatiesysteem worden onderzocht en het effect op de schattingen van verdamping worden geëvalueerd aan de hand van gegevens gemeten in het veld. In Hoofdstuk 3 worden het data-assimilatiesysteem en verschillende andere modelcomponenten in GLEAM verder verbeterd met het oog op een meer realistische voorstelling van het effect van het landoppervlak op het verdampingsproces. Hoofdstuk 3 stelt ook de resultaten voor van een uitgebreide validatie op wereldschaal van verdamping en bodemvocht, afgeleid uit deze nieuwe versie van GLEAM.

In Hoofdstuk 4 van dit proefschrift wordt het potentieel van GLEAM geëvalueerd om op hoge resolutie bodemvocht en verdamping af te leiden ter ondersteuning van lokaal waterbeheer en irrigatieplanning. In dit hoofdstuk wordt een pilootdataset van verdamping met een ruimtelijke resolutie van 100 m voor Nederland, Vlaanderen, en het westen van Duitsland gepresenteerd en gevalideerd met behulp van veldmetingen van bodemvocht en verdamping.

Het laatste doel van dit proefschrift is om de troeven van GLEAM te verkennen in twee *case studies* (Hoofdstukken 5 en 6). In Hoofdstuk 5 wordt GLEAM gebruikt als een hulpmiddel om de kwaliteit van *reanalysis* datasets te evalueren. Meer in het bijzonder wordt GLEAM ingezet (1) om de performantie van het landoppervlaktemodel in de *reanalysis* dataset te evalueren, en (2) om de kwaliteit van de atmosferische variabelen die verdamping beïnvloeden in de *reanalysis* dataset te beoordelen. Deze analyses bieden nuttige inzichten in de kwaliteit van de GLEAM datasets voor globale hydrologische en klimatologische studies. In Hoofdstuk 6, wordt de globale variabiliteit van verdamping over de laatste 40 jaar gelinkt aan interne klimaatvariabiliteit, voornamelijk als gevolg van de meest prominente klimaatmodi zoals de *El Niño Southern Oscillation* (ENSO).

Ten slotte vat Hoofdstuk 7 de belangrijkste conclusies uit dit proefschrift samen, alsook de belangrijkste beperkingen, en geeft het een potentiële piste weer om GLEAM verder te ontwikkelen, en om verder onderzoek naar de observatie van verdamping te sturen.

CHAPTER 1

Introduction

This chapter introduces the concept of terrestrial evaporation and frames its importance within the global hydrological cycle. It also aims at giving a non-exhaustive overview of various methods to measure and estimate terrestrial evaporation at different spatial and temporal scales. Finally, it provides the motivation, defines the objectives, and presents the structure of this dissertation.

1.1 Terrestrial evaporation

1.1.1 Terrestrial evaporation: an essential climate variable?

The hydrosphere of the Earth holds approximately $1.385 \cdot 10^{18} \text{ m}^3$ of water (Kundzewicz, 2008). About 97% of this total volume can be found in the oceans covering the largest part of our Earth surface, while most of the remaining volume is stored at the land surface in glaciers, groundwater reservoirs, lakes, and rivers. Only a very small fraction (less than 0.1%) is held in our atmosphere, either as water vapour mixed in the air, or as liquid droplets or ice crystals held in clouds (Kundzewicz, 2008). While the total volume of water in the hydrosphere can be assumed constant, the distribution of water across the different reservoirs – ocean, atmosphere, land, and reservoirs therein – is highly dynamic. This cycling of water within the Earth’s hydrosphere is known as the hydrological cycle (or water cycle), and the study of it at different scales is known as hydrology. Although such a cycle does not truly have a beginning, nor an end, vaporisation of water from the oceans and the land surface into the atmosphere is often considered as the starting point of the hydrological cycle. Atmospheric water vapour may subsequently condense and form clouds which produce precipitation, reaching both the oceans and the land surface. At the land surface, different processes re-distribute the water into several reservoirs such as groundwater, lakes, rivers, and back into the atmosphere through terrestrial evaporation. Taking these processes into account, together with the physical law of mass conservation, the terrestrial water balance at the catchment (or larger) scale can be written as:

$$\frac{ds}{dt} = P - E - Q, \quad (1.1)$$

where $\frac{ds}{dt}$ is the change in terrestrial water s (m) with respect to time t (s), and P , E , and Q are the volumes of precipitation, terrestrial evaporation, and river discharge, respectively; all expressed per unit area and per unit of time¹ ($\text{m} \cdot \text{s}^{-1}$).

Terrestrial evaporation (often referred to as *evapotranspiration*; Savenije, 2004) is the flux of water from the land surface into the atmosphere. The total flux consists of the vaporisation of water through plant stomata (transpiration), from water in the first few centimeters of the soil (bare soil evaporation), from open water such as lakes and rivers (open-water evaporation), from water captured by vegetation at e.g. leaves and stems (interception loss), and from snow and ice (sublimation). After precipitation, it is the second largest flux of

¹Note that hydrological fluxes are often expressed in different units of volume per unit area (e.g. mm) and time (e.g. day), depending on the magnitude of the fluxes and integration period considered. Units are always explicitly mentioned in this dissertation to avoid confusion, and the list of symbols provides the standard S.I. units for every variable, whenever applicable.

the terrestrial hydrological cycle; roughly about two thirds of the total volume of precipitation reaching the land surface is returned to the atmosphere via terrestrial evaporation, while only one third is discharged into the oceans via rivers (Dai *et al.*, 2009; Oki and Kanae, 2006; Dai and Trenberth, 2002; Church, 1996). Nevertheless, the exact total volume of evaporation from the continents into the atmosphere is hard to assess, mainly because of uncertainties in global data sets of terrestrial evaporation (Fisher *et al.*, 2017), and has therefore been subject to debate for over a decade now (Wild *et al.*, 2015; Wang and Dickinson, 2012). Depending on the method used to calculate the global magnitude of terrestrial evaporation, the region considered (e.g. permanently frozen land included or not), data processing, and ancillary data sets used, values may range between $55 \cdot 10^9 \text{ m}^3 \cdot \text{year}^{-1}$ and $80 \cdot 10^9 \text{ m}^3 \cdot \text{year}^{-1}$ (Miralles *et al.*, 2016; Wang and Dickinson, 2012, and references therein), making it one of the most uncertain components of the terrestrial branch of the hydrological cycle in terms of total magnitude and spatio-temporal variability.

Aside from returning water from the land surface into the atmosphere, terrestrial evaporation also consumes a substantial portion of the available energy at the land surface (Wild *et al.*, 2015; Wild and Liepert, 2010; Trenberth *et al.*, 2009), thereby linking the terrestrial water and energy cycles. This energy is used to re-arrange the water molecules leading to the change of phase from liquid (or solid) to gas, which requires approximately $2260 \cdot 10^3 \text{ J} \cdot \text{kg}^{-1}$ for liquid water under standard atmospheric conditions, a physical property known as the latent heat of vaporisation. The remaining energy available at the land surface is largely used to heat up the air and soil, while only minor portions are used by plants and animals. Note that the total amount of energy used to evaporate water from the land surface is referred to as the latent heat flux, while the energy used to heat up the air is called the sensible heat flux². Taking into account the physical law of energy conservation, the energy balance at the land surface can thus be approximated as (ignoring biological energy consumption through photosynthesis and advection of energy):

$$\frac{d\epsilon}{dt} = R_n - \lambda \rho E - H - G, \quad (1.2)$$

where $\frac{d\epsilon}{dt}$ is the change in terrestrial energy storage ϵ ($\text{J} \cdot \text{m}^{-2}$) with respect to time, R_n is the surface net radiation ($\text{W} \cdot \text{m}^{-2}$), being the balance of incoming radiation from the atmosphere and outgoing radiation from the land surface, λ is the latent heat of vaporisation ($\text{J} \cdot \text{kg}^{-1}$), ρ is the density of water ($\text{kg} \cdot \text{m}^{-3}$),

²In this dissertation, the terms latent heat flux and terrestrial evaporation will be used interchangeably, depending on the context. As both the latent and sensible heat flux are turbulent fluxes, the latter term will also be used occasionally to refer to them.

$\lambda\rho E$ is the surface latent heat flux³ ($\text{W}\cdot\text{m}^{-2}$), H is the surface sensible heat flux ($\text{W}\cdot\text{m}^{-2}$), and G is the ground heat flux ($\text{W}\cdot\text{m}^{-2}$). Using an atmospheric model, Shukla and Mintz (1982) concluded that the Northern Hemisphere would be on average 15 to 25°C warmer if terrestrial evaporation would be zero, highlighting the importance of this process to keep the air temperature at reasonable levels for life on Earth.

Terrestrial evaporation is also closely coupled to the carbon cycle at the land surface through the synchronisation of photosynthesis and transpiration (Gentine *et al.*, 2019). The latter process is known to contribute most to terrestrial evaporation at the global scale (Schlesinger and Jasechko, 2014; Jasechko *et al.*, 2013). During photosynthesis, which requires the plant to open its stomata in order to capture atmospheric carbon dioxide molecules (CO_2), water vapour escapes via these same openings in the plant leaves (transpiration); in response, plants extract water from the soil to replenish the loss of water via transpiration (Collatz *et al.*, 1991). By assimilating CO_2 in its organic tissues as carbohydrates and respiring them again to meet the plants demand for energy – releasing back CO_2 into the atmosphere – plants might either act as a carbon sink or stock at the land surface, highlighting their role in balancing rising atmospheric CO_2 levels due to anthropogenic activity (Baccini *et al.*, 2017; Reichstein *et al.*, 2013; Pan *et al.*, 2011; Beer *et al.*, 2010). However, the extent to which plants open their stomata to capture CO_2 – also known as stomatal conductance⁴ – heavily depends on environmental conditions such as the availability of water in the soil to replenish their water content, and the biophysical state of the plant (Stocker *et al.*, 2019; Collatz *et al.*, 1991), resulting in a strong correlation of terrestrial carbon storage and regional climatic conditions (Claessen *et al.*, 2019; Beer *et al.*, 2010; Nemani, 2003). In addition, changes in the atmospheric composition due to increasing CO_2 concentrations alter the surface radiation budget, directly affecting terrestrial evaporation and the so-called intensity of the hydrological cycle (Wild and Liepert, 2010; Wild *et al.*, 2008; Huntington, 2006). As such, terrestrial evaporation is paramount in mediating the effect of rising atmospheric CO_2 concentrations on the terrestrial hydrological cycle and our water resources in general (Berg and Sheffield, 2019a; Fowler *et al.*, 2019; Ukkola *et al.*, 2015).

Terrestrial evaporation is thus a crucial process in the climate system and the primary variable necessary to properly manage our water resources (Hagemann

³Note that the symbol λE is often used to denote the surface latent heat flux. However, given that E is expressed here as a volume of liquid water per unit area and per unit of time, ρ is needed to convert that volume to an equivalent mass of water prior to transforming it to a unit of energy.

⁴Conductance is a measure related to the ease at which water vapour may flow through a medium (in the current context being plant stomata) and is inversely and linearly proportional to resistance. In this dissertation, both resistance and conductance will be used interchangeably, depending on the context.

et al., 2013) and optimise irrigation systems (Allan *et al.*, 1998). By linking the terrestrial carbon and water cycles, it also serves as a diagnostic of vegetation activity (Fisher *et al.*, 2011) and partly controls atmospheric CO₂ concentrations (Reichstein *et al.*, 2013). Due to its consumption of energy, it also affects the cycling of energy in the atmosphere, ultimately regulating air temperature by altering the ratio of the sensible and latent heat fluxes (Miralles *et al.*, 2014, 2012; Seneviratne *et al.*, 2010). Finally, by supplying water vapour to the atmosphere, terrestrial evaporation also affects the atmospheric moisture content, thereby influencing both local and remote cloud formation (Teuling *et al.*, 2017) and precipitation (Taylor *et al.*, 2012). This bi-directional link between the land surface and the atmosphere is often referred to as land–atmosphere feedback, and has been identified as a critical process in the occurrence and evolution of droughts and heatwaves (Miralles *et al.*, 2019, 2014; Seneviratne *et al.*, 2010), especially in regions where meteorological conditions are strongly dependent on convection (Roundy *et al.*, 2013). As such, terrestrial evaporation also plays a key role in the occurrence of hydro-meteorological extremes, thereby affecting fresh water availability (Keune and Miralles, 2019), food production (Sheffield *et al.*, 2018), and the development of extreme air temperatures (Schumacher *et al.*, 2019).

Being a nexus between different bio-geochemical cycles and a crucial variable helping to characterise the state of the climate system and its dynamics, the surface latent heat flux – together with the surface sensible heat flux – was recognised by the World Meteorological Organisation (WMO) as an Essential Climate Variable (ECV) under the Global Climate Observing System (GCOS) program in 2017⁵. Thereby, WMO acknowledges its importance to support the work of the Intergovernmental Panel on Climate Change (IPCC) and the United Nations Framework Convention on Climate Change (UNFCCC) in providing policymakers accurate information about climate change and its impacts on our Earth system.

1.1.2 Physics of terrestrial evaporation

Although the first thoughts on terrestrial evaporation probably date back to the Ancient Greeks, the theoretical foundations to physically describe the evaporation process and to develop mathematical equations to estimate evaporation from environmental variables have only been established two centuries ago by scientists such as John Dalton, Howard L. Penman, and John L. Monteith. Dalton was the first one to formally derive an equation

⁵An ECV is a physical, chemical, or biological variable (or a group of linked variables) that critically contributes to the characterisation of Earth’s climate and information on these variables is deemed necessary to support the work of the IPCC and UNFCCC. More information can be found at <https://gcos.wmo.int/en/essential-climate-variables>; last visit: 16 November 2019

to estimate evaporation from a free evaporating water surface based on wind speed and Vapour Pressure Deficit (VPD; Dalton, 1802). Acknowledging the importance of wind – which strongly determines the aerodynamic resistance to water vapour; i.e. the resistance of the atmosphere to transport of water vapour – in the evaporation process, research in the following decades mainly focused on deriving improved empirical functions describing the effect of wind. However, only in 1877 Boussinesq formalised the concept of atmospheric turbulence, and the movement of water vapour from the land surface into the atmosphere was acknowledged to take place under the form of turbulent transport (i.e. by means of large-scale eddies of varying size) rather than molecular diffusion. In 1926, Bowen recognised the available energy at the land surface as an important driver of evaporation and derived a method to estimate evaporation from lakes (Bowen, 1926). In essence, the method combined the energy-balance equation (Equation 1.2) and equations describing the bulk transfer of heat and water vapour based on the eddy-diffusivity concept introduced by Boussinesq, leading to the well-known Bowen ratio method (Section 1.1.3). Penman further elaborated on the work of Bowen to derive a more advanced mathematical formulation describing terrestrial evaporation based on net radiation, air temperature, wind speed, and VPD (Penman, 1948). Around the same time, Monin and Obukhov (1954) introduced their correction functions for atmospheric stability to the eddy-diffusivity equations, leading to the most complete description of the evaporation process as a turbulent transfer of water vapour from the land surface into the atmosphere at that time.

However, up to 1950, only atmospheric parameters influencing terrestrial evaporation had been considered and the land surface control on the flux had not yet been recognised. Existing theories at that point thus only allowed the calculation of some form of atmospheric demand for water, often referred to as potential evaporation⁶ (Fisher *et al.*, 2011; Ludovic *et al.*, 2005; Thornthwaite, 1948). Monteith elaborated on Penman’s equation and included the land surface control on the flux in the formula, leading to the most renowned equation to estimate terrestrial evaporation from a natural surface known as the Penman-Monteith equation (Monteith, 1965). The equation accounts for both the atmospheric demand for water (i.e. the potential to evaporate water) and the ease to supply it from the surface (i.e. how much water is the

⁶Note that no unique definition of potential evaporation exist and that different definitions are used across disciplines (Maes *et al.*, 2019). In this dissertation, potential evaporation is defined as the maximum evaporation rate possible under given meteorological conditions and a patch of land whether or not covered with vegetation. Hence, it partly takes into account the land surface control through (1) its effect on atmospheric properties such as aerodynamic resistance, and (2) the maximum surface conductance of the land cover under consideration (i.e. no evaporative stress). The land surface control on terrestrial evaporation will in turn be defined as the ability of the land surface to supply the water demanded by the atmosphere under actual conditions (i.e. including evaporative stress).

surface prone to lose) and thus calculates the “actual” terrestrial evaporation (hereafter referred to as terrestrial evaporation). Estimating the land surface resistance to evaporation is challenging and requires detailed information on vegetation state, the sensitivity of vegetation to environmental stressors, soil properties, etc., which resulted in a plethora of empirical equations to estimate this resistance (e.g. Stewart, 1988; Ball *et al.*, 1987; Jarvis *et al.*, 1976).

Given the strong demands in terms of meteorological data to properly apply the Penman-Monteith equation, several empirical formulas describing terrestrial evaporation have been developed over the last decades (e.g. Fisher *et al.*, 2011; Ludovic *et al.*, 2005, for a review of methods). The Priestley and Taylor equation (Priestley and Taylor, 1972) is probably the best known and is essentially a simplified version of the Penman-Monteith equation, only relying on measurements of surface net radiation and air temperature. The equation does not explicitly consider wind speed and introduces an empirical, vegetation-dependent parameter to account for the aerodynamic effects on terrestrial evaporation. However, the Priestley and Taylor equation has been derived for well-watered grasslands and it thus requires modifications for the estimation of actual evaporation (Chapters 2 and 3). Another, even simpler, yet widely-used equation is the one from Thornthwaite (1948). The Thornthwaite equation also ignores the land surface control on terrestrial evaporation and has been applied in many studies and applications because of its simplicity, and its dependence on measurements of air temperature alone.

The mathematical formulations discussed above essentially allow the estimation of terrestrial evaporation at any temporal and spatial scale, whenever the required input data are available, and the physical assumptions are met (Shuttleworth, 2007). As such, they have been implemented in several modelling frameworks varying in their complexity and primary objective (e.g. Sellers *et al.*, 1997, for an early review of such approaches). Hydrological models are relatively simple and aim at the accurate estimation of all hydrological fluxes (including terrestrial evaporation), but generally with a clear focus on simulating river discharge (e.g. Gao *et al.*, 2010; Ludovic *et al.*, 2005). Land surface models are typically more complex and aim to describe the terrestrial water, carbon, and energy cycles (e.g. Le Quéré *et al.*, 2018, for an overview). Such models have been coupled with atmospheric models and data assimilation systems ingesting huge amounts of atmospheric observations, producing so-called climate reanalyses (e.g. Hersbach *et al.*, 2018; Gelaro *et al.*, 2017; Dee *et al.*, 2011), or have been forced offline with atmospheric forcing from reanalyses – i.e. not coupled to an atmospheric model – to produce stand-alone land surface reanalysis data sets (e.g. Albergel *et al.*, 2018; Reichle *et al.*, 2017; Balsamo *et al.*, 2015). Land surface models have also been embedded within climate models – which model physical processes in the atmosphere, ocean, and land – to represent the interaction between the land surface and the

atmosphere, which has deemed essential for improving the accuracy of climate projections (Dirmeyer *et al.*, 2018; Santanello *et al.*, 2018). Finally, Earth system models aim at describing all relevant climate processes on Earth, including physical, biological, and chemical processes, and essentially implement our entire current knowledge of the Earth system into an abstract mathematical model (Heavens *et al.*, 2013). Such models are generally considered being the most complete tools describing our Earth system, but are very complex and computationally demanding. Although such mathematical models have been the only source of truly global information on terrestrial evaporation for many years, their primary objective has never been to produce accurate estimates of the flux (Mueller *et al.*, 2013; Jiménez *et al.*, 2011). This strongly fostered research over the last decade to develop algorithms to derive data sets of terrestrial evaporation at the global scale from satellites (Section 1.1.4).

1.1.3 Terrestrial evaporation from in situ observations

Unlike precipitation and river discharge, the other two major fluxes in the terrestrial hydrological cycle (Section 1.1.1), evaporation is relatively difficult to measure in the field, and several techniques have been developed over the last decades (e.g. Wang and Dickinson (2012) and Shuttleworth (2007) for a review of methods). These techniques typically measure either the total flux or one of its components, and their spatial representativeness ranges from a single point to the scale of a watershed. Despite the fact that such measurements are prone to errors due to e.g. sensor malfunctioning, natural disturbances, erroneous installation of sensors, or extreme weather conditions, measuring evaporation in the field still presents the most accurate means to evaluate the variability and magnitude of the flux at the local scale. Below, the most commonly-used measurement techniques are briefly discussed.

The most established and widely-used technique – and arguably the only approach that measures the surface latent heat flux (and sensible heat flux) directly with a minimal number of theoretical assumptions – is the eddy-covariance method. The method relies on calculating correlations between fluctuations in wind speed, humidity, and temperature in the lower part of the troposphere known as the atmospheric boundary layer. Measurements of these variables are typically made at temporal frequencies higher than 10 Hz to capture the strong temporal fluctuations in these atmospheric properties, which requires relatively expensive sensors (Wang and Dickinson, 2012). Given that the eddy-covariance method is able to independently derive both the surface sensible and latent heat fluxes, the energy-balance closure at the site can be easily calculated when measurements of the soil heat flux and surface net radiation are available as well (Equation 1.2). Such calculations have revealed that the turbulent fluxes are typically underestimated by the eddy-covariance method (Beer *et al.*, 2010; Wilson *et al.*, 2002), mostly affecting the latent heat

flux, and different approaches to correct for this underestimation have been proposed (e.g. Wang and Dickinson, 2012, for a review of methods). Despite this shortcoming, the eddy-covariance approach is considered to be one of the most accurate techniques to measure the surface turbulent fluxes. As a result, measurements are intensively used by the scientific community to validate estimates of terrestrial evaporation derived from different methods. In recent years, much effort has also been put on compiling consistent data sets of eddy-covariance measurements covering the entire globe, such as the FLUXNET initiative (Baldocchi *et al.*, 2001), the National Ecological Observatory Network (NEON), or the Integrated Carbon Observation System (ICOS), which are warmly-welcomed by the scientific community. Eddy-covariance data are also extensively used in this dissertation as described in Sections 2.3.2, 3.3.2, 4.2.2, and 5.2.2. Note that the issue of the underestimation of the latent heat flux by eddy-covariance systems and a potential solution are briefly explored in Section 2.5.3. However, as correction techniques require the availability of measurements of net radiation and the ground heat flux, data that are not available at every in situ site⁷, only non-corrected measurements are used in the remaining chapters of this dissertation.

The Bowen ratio technique is another popular method to estimate the turbulent fluxes in the field. The Bowen ratio is defined as the ratio of the sensible and latent heat flux, and can be theoretically related to vertical differences in air temperature and humidity near the land surface when the aerodynamic resistance for heat and moisture transport can be assumed equal (Bowen, 1926). The technique uses measurements of vertical gradients in air temperature and humidity near the surface to calculate the Bowen ratio, and measurements of surface net radiation and the ground heat flux, to solve the surface energy balance (Equation 1.2) for the turbulent fluxes. The method is relatively cheap compared to an eddy-covariance installation, but it relies on strong assumptions that are not necessarily met in nature, and it generally fails when the near-surface atmosphere is relatively stable (i.e. only small gradients prevail and measurement errors become important; Angus and Watts, 1984). Small gradients also often occur over forests because their high aerodynamic roughness results in high turbulent fluxes, making the technique less reliable over these land cover types (Shuttleworth, 2007). Note that some of these problems might be circumvented by making use of more innovative measurement techniques deriving high-resolution vertical profiles of air temperature (better known as distributed temperature sensing) and humidity using for instance fibre optic cables rather than the more traditional Bowen ratio measurement at two fixed heights above the land surface (Schilperoort *et al.*, 2018; Euser *et al.*, 2014). Networks of Bowen ratio stations – such as the Atmospheric Radiation

⁷For the largest sample of sites used in this dissertation (Chapter 5; Table A.4), these measurements are only available at approximately 65% of the sites.

Measurement (ARM) network⁸ – have been established over the last decade because of its low maintenance cost and relatively easy measurement strategy, and are mainly used in agricultural applications.

As both the Bowen ratio and eddy-covariance technique use measurements of atmospheric properties that are influenced by processes in a certain surrounding region, better known as the footprint (or fetch) of the sensor, their estimates of the turbulent fluxes are in turn representative for that same region. This area typically covers a few hectares and is in principle located upwind of the measurement station, but the actual size and location of the footprint strongly depends on the atmospheric conditions and the land surface properties, and different algorithms have been proposed to get a sense of this footprint (Lee *et al.*, 2004).

Another widely-used approach in agriculture to estimate terrestrial evaporation is to monitor the loss of water from a tank or pan. By accurately measuring this loss and balancing this with the input (rainfall), one can calculate the net loss due to evaporation. However, in reality this is only a poor proxy of the true evaporation from natural surfaces such as an agricultural field, as water is generally not endlessly available to plants as in an evaporation pan, nor will atmospheric conditions be the same as plants strongly affect the near-surface air flow and energy balance, directly influencing the potential to evaporate water. As such, crop- and environmental-specific empirical parameters are typically required to account for these differences and to obtain an estimate of terrestrial evaporation from the agricultural field of interest. Atmometers somehow try to circumvent this problem by measuring the loss of water from a small porous cup or reservoir covered with a porous fabric mimicking the plant leaf. However, empirical conversion factors are still needed because of the unlimited supply of water from the reservoir, and the obvious difference in physical properties between actual plant tissues and the atmometer.

A more reliable approach is to use lysimeter containers and calculate the loss of water due to evaporation based on the water balance of the container. Lysimeters are containers filled with soil (and natural vegetation) in which continuous measurements of in- and outgoing water fluxes are made. The aim is to realistically simulate natural conditions, and the system should thus be carefully designed and installed. Under these circumstances, weighable lysimeters – which measure the mass of the entire container with a typical temporal resolution of 30–60 minutes – provide the most accurate estimate of terrestrial evaporation at the local scale (Holmes, 1984). However, this type of system is expensive to install and maintain and are typically only used for scientific purposes, e.g. to validate alternative measuring techniques or to advance our process understanding (Perez-Priego *et al.*, 2017; Gebler *et al.*, 2015).

⁸More information can be found at <https://www.arm.gov/>; last visit: 16 November 2019.

The main issue with the above-mentioned techniques is that their estimates are only representative for a rather small area, essentially ranging from a point (e.g. atmometer measurements) to a few hectares (e.g. eddy-covariance measurements). A more recent approach to measure terrestrial evaporation is to make use of scintillimeters (De Bruin *et al.*, 1995), which measure anomalies (scintillations) in the electromagnetic field between a transmitter and receiver that are typically related to the surface sensible heat flux. An estimate of the latent heat flux may then be obtained by using the energy-balance equation (Equation 1.2) in combination with measurements of the ground heat flux and surface net radiation. Depending on the distance between the transmitter and receiver, estimates from scintillimeters may be representative for areas covering several squared kilometres, making them particularly useful to validate model- and satellite-based estimates of terrestrial evaporation (Samain *et al.*, 2012). Also highly-accurate gravimetric measurements have been proven to be appropriate to estimate terrestrial evaporation over relatively large areas (Van Camp *et al.*, 2016). With this technique, changes in gravity are typically related to changes in water storage, after correcting for the impact of extra-terrestrial bodies such as the Sun. By taking into account the effect of subsurface flow and precipitation on terrestrial water storage, changes in gravity can be exclusively related to the loss of water from the system via terrestrial evaporation (Van Camp *et al.*, 2016). Yet an alternative means to obtain estimates of the flux over larger areas is to calculate it from the terrestrial water-balance equation (Equation 1.1) at e.g. the catchment or continental scale. Given that river discharge and precipitation can typically be measured with higher confidence, Equation 1.1 can be used to estimate terrestrial evaporation when changes in storage can be measured or ignored (Wang and Dickinson, 2012). Note that changes in storage are often ignored, but that it is only valid when sufficiently large time periods are considered (Section 5.2.3).

Finally, there is a wide variety of methods that aim to measure or estimate the separate components of terrestrial evaporation ranging from plant-based measurements of sap flow to the use of bio-physical or statistical models (e.g. Talsma *et al.*, 2018a; Schlesinger and Jasechko, 2014, for an overview of methods). At the plant level, measurements of water vapour in chambers installed on plants, leaf-scale measurements of water vapour exchange between plant and atmosphere, and measurements of sap flow velocity may be linked to transpiration. While the latter technique is very plant-specific (sap flow velocity strongly depends on plant age and physiological state), and is thus difficult to upscale to e.g. a forest stand or a catchment, measurements are increasingly being used in large-scale studies, mainly to assess the contribution of transpiration to the total flux of terrestrial evaporation (Schlesinger and Jasechko, 2014; Moran *et al.*, 2009), or to validate estimates of transpiration from models (Talsma *et al.*, 2018a). This is also fostered by efforts to compile consistent data sets of

sapflux measurements, such as SAPFLUXNET (Poyatos *et al.*, 2016). Based on the principle that lighter water isotopes evaporate more easily than heavier ones, analysis of the isotopic composition of different water compartments in a catchment such as soil, leaf, and streams, also provides a means to estimate the separate components of terrestrial evaporation. Due to the preferential evaporation of light water isotopes, leaf water may for instance become enriched by heavy water isotopes. Analysing the isotopic composition of leaf and soil water may therefore provide insights on transpiration (Farquhar *et al.*, 2007). Finally, interception loss is relatively difficult to measure directly and is typically derived by solving the canopy water balance based on measurements of above-canopy rainfall, direct throughfall, and stemflow (Miralles *et al.*, 2010; Lloyd and Marques, 1988; Gash and Stewart, 1977).

1.1.4 Terrestrial evaporation from satellite observations

Over the last decades, several satellites have been launched with the primary objective to monitor atmospheric and land surface variables from space (McCabe *et al.*, 2017a). Figure 1.1 shows an overview of the Earth observation programs of the European Space Agency (ESA) and the National Aeronautics and Space Administration (NASA) to illustrate the plethora of satellites available for Earth system monitoring. While many essential surface climate variables such as soil moisture (Kerr *et al.*, 2012), precipitation (Huffman *et al.*, 2007), land surface temperature (LST; Zhengming and Dozier, 1996), or vegetation state (Barnsley *et al.*, 2004) can be retrieved from such satellite-based measurements in a rather direct way (Figure 1.1), terrestrial evaporation cannot be “seen” from space as it does not affect the electromagnetic waves reflected at or emitted from the Earth’s surface. Although satellites provide a valuable means to retrieve land surface information at the global scale with an acceptable temporal resolution, researchers have thus been forced to combine remotely-observable variables related to the evaporation process in physical, process-based, or statistical models to derive terrestrial evaporation from remote sensing observations (Zhang *et al.*, 2016a).

The first attempts used LST retrieved from remote sensors in combination with measurements (or estimates) of near-surface air temperature to calculate the sensible heat flux based on the eddy-diffusivity concept describing the bulk transport of heat (Section 1.1.2). Subsequently, the latent heat flux may be estimated as the residual of the energy balance (Equation 1.2) when observations (or estimates) of net radiation and the ground heat flux are available as well (Kalma *et al.*, 2008). Methods relying on this approach are also known as surface energy balance (SEB) algorithms, and mainly differ in the way they parameterise the atmospheric resistance to heat transfer (Zhang *et al.*, 2016a; Kalma *et al.*, 2008). One-source SEB algorithms treat the land surface as one homogeneous patch and do not distinguish between transpiration and bare

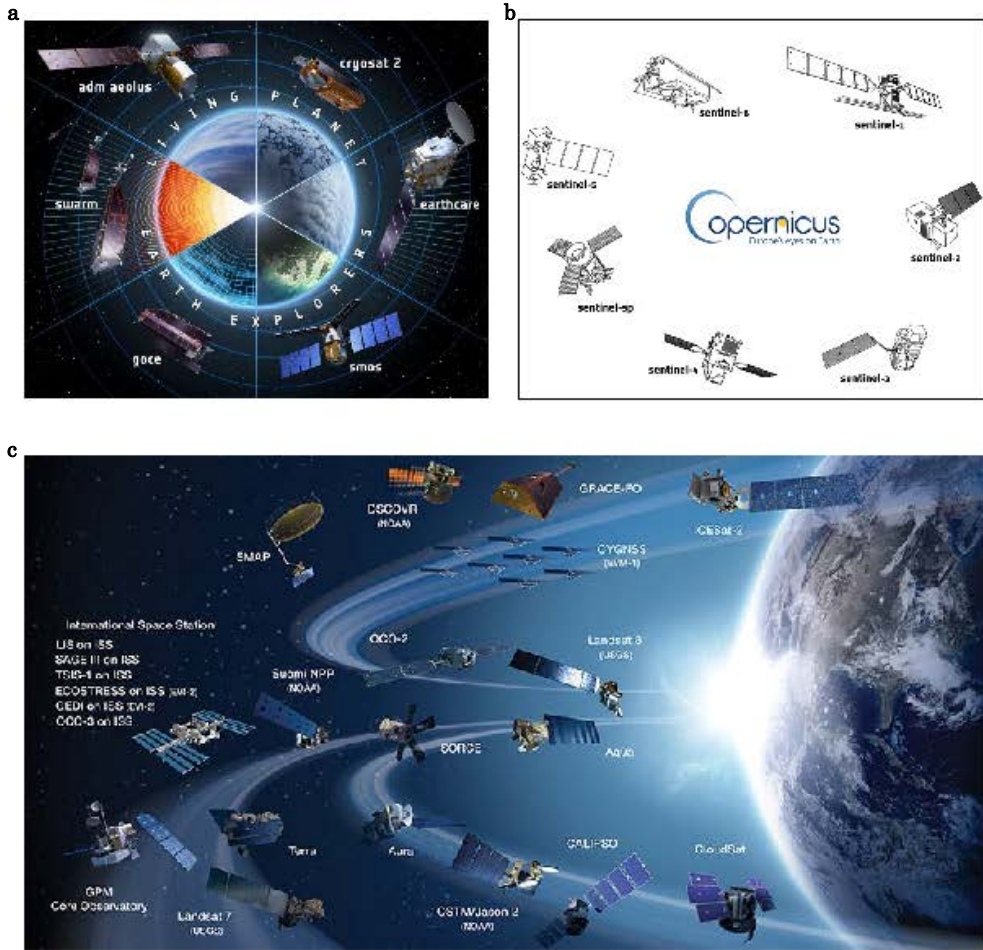


Figure 1.1: Overview of (a) the Earth Explorers program from ESA, (b) the Copernicus program from ESA, and (c) NASA's Earth observing system. Figures reprinted from (a) "Earth observation missions" (article at <http://www.esa.int/>; last visit: 24 November 2019), (b) Kyrlyuk and Kratzer (2019), and (c) "NASA's Earth Observing System" (article at <https://eospsso.nasa.gov/>; last visit: 16 November 2019).

soil evaporation; although both processes differ inherently in their physical and biological mechanisms. The first one-source SEB models were already described in the early 90's by Kustas (1990) and Kalma and Jupp (1990) to estimate terrestrial evaporation at field scales using LST derived from thermal infrared (TIR) cameras mounted on meteorological towers. Further advances in the field led to algorithms able to calculate the latent heat flux from actual satellite data such as the Surface Energy Balance Algorithm for Land (SEBAL) from Bastiaanssen *et al.* (1998), and the Surface Energy Balance System (SEBS) from Su (2002). As opposed to one-source SEB algorithms, two-source algorithms

separately consider the contribution of soil and vegetation to the total latent heat flux. Arguably, the models described by Kustas (1990) and Norman *et al.* (1995) are the first applications of such two-source models. Two-source SEB models have also been implemented more recently in frameworks that can be applied on satellite-based retrievals of LST such as the Atmosphere–Land EXchange Inverse (ALEXI) model described in Anderson *et al.* (1997) and the more advanced Disaggregated ALEXI model from Norman *et al.* (2003).

Given that SEB models first calculate the sensible heat flux using the vertical gradient in temperature, and that this information is not directly available from satellites, they typically need to rely on assumptions about the change of temperature with height above the surface (Kalma *et al.*, 2008). Estimates of the latent heat flux thus strongly depend on the validity of these assumptions. On top of that, they are highly sensitive to the accuracy of LST retrieved from the satellite system (Zhang *et al.*, 2016a), as the difference in LST and near-surface air temperature may be small as compared to the measurement error (Timmermans *et al.*, 2007). In addition, LST is generally derived from measurements in the TIR spectrum, making it susceptible to clouds and hampering the estimation of the turbulent heat fluxes under these conditions. While this issue may be avoided by using LST derived from microwave measurements (Holmes *et al.*, 2016), this supersedes the main advantage of SEB-based methods of providing estimates of the turbulent fluxes with high spatial resolution (generally better or equal to 10 m). SEB-based methods thus excel in their ability to derive terrestrial evaporation at both high spatial (up to 1 m using LST derived from sensors on drones) and temporal resolution (up to several minutes using LST derived from geostationary imagery). However, given that they require information that is not easily measured from space (Tarpley, 1994), together with assumptions on (or local calibration of) the aerodynamic resistance and vertical gradient of air temperature, difficulties arise to derive truly global fields of terrestrial evaporation using such methods (Jiménez *et al.*, 2011).

Consequently, several studies have explored alternative strategies in recent years. Next to climate reanalyses (e.g. Hersbach *et al.*, 2018; Gelaro *et al.*, 2017; Dee *et al.*, 2011), hydrological models (e.g. Gao *et al.*, 2017; Ludovic *et al.*, 2005), and land surface models (Albergel *et al.*, 2018; Reichle *et al.*, 2017; Le Quéré *et al.*, 2018; Balsamo *et al.*, 2015; Ghilain *et al.*, 2011) partly driven or steered by satellite data (Section 1.1.2), different algorithms specifically designed to estimate terrestrial evaporation have also been developed over the last years. Given the physical background of the Penman-Monteith equation (Section 1.1.2), its use to derive terrestrial evaporation from satellite measurements is tempting, but not straightforward, as the correct application requires the parameterisation of both the surface and aerodynamic resistance. Mu *et al.* (2007) and Mu *et al.* (2011) developed a framework using the Penman-Monteith equation to estimate terrestrial evaporation from a vari-

ety of geophysical variables derived from the MODerate-resolution Imaging Spectroradiometer (MODIS) instrument onboard Terra and Aqua, well known as the MOD16 algorithm. The method relies on a combination of empirical vegetation-dependent constants and stress functions depending on temperature and VPD to estimate the surface resistance. Also Zhang *et al.* (2015, 2010) and Leuning *et al.* (2008) proposed a method based on the Penman-Monteith equation, both introducing new formulations to estimate surface resistance; however, they also strongly rely on a local calibration of model parameters against eddy-covariance data.

Except for the need to calibrate model parameters, methods based on the Penman-Monteith equation generally also require forcing data that cannot be easily measured from space, such as wind speed or VPD. These forcing data are then typically sourced from atmospheric reanalyses, making the estimates of terrestrial evaporation not truly satellite-based and susceptible to uncertainties in the reanalyses (Jiménez *et al.*, 2011). The use of the more simple, yet empirical, Priestley and Taylor equation (Section 1.1.2) may overcome the use of reanalysis data because it only requires air temperature and surface net radiation as inputs, both available from satellite measurements (Miralles *et al.*, 2011b). Arguably the most well-known global-scale algorithms are the ones developed by Fisher *et al.* (2008) and Miralles *et al.* (2011b), known as the Priestley Taylor Jet Propulsion Laboratory (PT-JPL) algorithm and the Global Land Evaporation Amsterdam Model (GLEAM), respectively. Both methods first calculate potential evaporation using the Priestley and Taylor equation, but differently constrain the flux using empirical stress functions taking into account the effect of the land surface on the evaporation process. The use of the Priestley and Taylor equation in combination with these empirical stress functions makes these methods a priori less physically-based, yet they are particularly suitable for global scales, and rely to the largest extent on satellite-based data to estimate terrestrial evaporation (Jiménez *et al.*, 2011). Note that GLEAM will be the model that is mostly used in this dissertation and that an in-depth description of the model can be found in Chapters 2 and 3.

Next to physical and process-based models described in the previous paragraphs, researchers have also developed statistical methods, typically trained on eddy-covariance data, to derive terrestrial evaporation from satellite data (e.g. Jung *et al.*, 2019; Alemohammad *et al.*, 2017; Jiménez *et al.*, 2009; Jung *et al.*, 2009) or to merge independent data sets of terrestrial evaporation aiming to combine the strengths of different methods (e.g. Hobeichi *et al.*, 2018; Jiménez *et al.*, 2018; Yao *et al.*, 2017). Arguably one of the most well-known data sets is the global FLUXCOM data set (Jung *et al.*, 2019) providing estimates of the turbulent fluxes, as well as their main atmospheric drivers, by merging eddy-covariance and satellite-based data using machine learning algorithms. As the method makes use of an ensemble of machine learning algorithms, it

provides relatively accurate estimates of terrestrial evaporation, next to an estimate of its uncertainty (Jung *et al.*, 2019) by exploiting the advantages of having global and coarse satellite-based data and reliable, but globally-sparse, eddy-covariance measurements.

Given the plethora of methods to estimate terrestrial evaporation from remote sensing data and the importance to derive global and consistent observational data sets of the variable, many studies have recently compared the potential of these methods (Pan *et al.*, 2019; Gomis-Cebolla *et al.*, 2019; Talsma *et al.*, 2018a; McCabe *et al.*, 2016; Michel *et al.*, 2016; Miralles *et al.*, 2016; Mueller *et al.*, 2013; Jiménez *et al.*, 2011). Conclusions of such studies generally point towards substantial differences in accuracy between the different algorithms and strong disparity on the partitioning of total terrestrial evaporation into its components (Talsma *et al.*, 2018a; Miralles *et al.*, 2016).

1.2 Motivation and objectives of this dissertation

Despite the importance of terrestrial evaporation, the high level of attention the variable achieved in recent years, and scientific advances made to observe or estimate the variable over the last decade, still today, it remains one of the most uncertain and elusive variables in (global) hydrology (Fisher *et al.*, 2017; McCabe *et al.*, 2017a; Harrigan and Berghuijs, 2016; Dolman *et al.*, 2014; Dolman and de Jeu, 2010). Many recent studies have demonstrated the need for correct information on the variability and magnitude of terrestrial evaporation at different spatial and temporal scales; the latter depending on the application. Otkin *et al.* (2016) and Sheffield *et al.* (2012) for instance concluded that droughts – which are projected to occur more often and to intensify due to our changing climate – could be better monitored and forecasted in case drought indices are used that properly take into account terrestrial evaporation. The latter is key, as droughts may have an enormous socio-economical impact by affecting crop yields, resulting in huge economic losses for farmers, and potential food shortages (Sheffield *et al.*, 2018; Funk and Brown, 2009). In addition, droughts may endanger drinking water availability and exacerbate air temperatures, eventually resulting in lethal temperatures for humans (Schumacher *et al.*, 2019). Also crop monitoring and forecasting in general could benefit substantially from accurate data on terrestrial evaporation (Huang *et al.*, 2019). Hence, the importance of data on terrestrial evaporation is paramount for local and regional-scale water resources management and irrigation planning in order to secure the availability of fresh water and food (e.g. Keune and Miralles, 2019; Orth and Destouni, 2018; Anderson *et al.*, 2012; Farahani *et al.*, 2007). Also studies assessing the global terrestrial water, carbon, or energy budget, and their temporal dynamics, are typically hampered by uncertainties in data sets of the surface turbulent fluxes (Le Quéré *et al.*, 2018; Zhang *et al.*,

2018). Such studies, however, are crucial to guide climate policy and to better project future climate and its impacts on society (Le Quéré *et al.*, 2018).

The main reason for the uncertainty is that it is particularly challenging to accurately monitor the flux with the required spatio-temporal detail (Fisher *et al.*, 2017; Harrigan and Berghuijs, 2016). At the very local scale, terrestrial evaporation is relatively easy to measure (Section 1.1.3), but it is not straightforward to spatially interpolate these in situ measurements to obtain information representative of larger areas (e.g. watersheds). At the regional scale, SEB-based algorithms (Section 1.1.4) may provide estimates of terrestrial evaporation with both high spatial and temporal detail, but problems arise when meteorological conditions are sub-optimal for the retrieval of LST in the TIR spectrum (Holmes *et al.*, 2016). Finally, at the global scale, algorithms exist to derive terrestrial evaporation from satellite-based measurements, but little agreement on the global-scale magnitude and variability is found between data sets derived using these methods, mainly due to different approaches to model the biotic control on the flux, and the use of uncertain forcing data (McCabe *et al.*, 2017a; Miralles *et al.*, 2016). In addition, global-scale data sets of terrestrial evaporation are typically only available at coarse spatial resolution as a result of the limited availability of high resolution input data sets from satellites, and are thus less useful for local or regional-scale water management (McCabe *et al.*, 2017a).

Fisher *et al.* (2017) compiled a list of ten critical questions within the fields of climate, agriculture, hydrology, and ecology that, to date, cannot be properly answered due to our limited knowledge of terrestrial evaporation. Some of these questions relate to our abilities to secure food and fresh water availability in current times such as: What is the timing of water use among ecosystems, and how does that vary diurnally, seasonally, and annually? How do changes in plant water availability, access, use, and stress regulate photosynthesis and productivity? How can information on terrestrial evaporation be applied to optimize sustainable water allocations, agricultural water use, food production, ecosystem management? Other questions are more important to help guiding climate policy and to develop mitigation and adaptation strategies: How are natural and managed ecosystems responding to changes in climate and water availability? How is terrestrial evaporation partitioned into transpiration, soil evaporation, and interception evaporation, and how are these components differentially impacted by a changing temperature, CO₂, and hydrologic regime? How do changes in terrestrial evaporation amplify or dampen climate feedbacks, land-atmosphere coupling, and hydro-meteorological extremes at local to regional scales? To be able to answer these questions as soon as possible, Fisher *et al.* (2017) also suggested an ambitious path forward, highlighting the need for more accurate data sets of terrestrial evaporation (preferably less than 10% relative error), with higher spatial (preferably better than

100 m) and temporal detail (sub-daily), covering both longer time periods (multi-decadal) and larger spatial domains (global land surface). As such, the paper called for prioritising scientific research on terrestrial evaporation and investments to enhance our capabilities to monitor the flux at better spatio-temporal resolutions and with higher accuracy. Also the World Climate Research Programme (WCRP) recently highlighted in a white paper the need to improve data sets of the surface turbulent fluxes, to harmonise measurement networks, and to integrate knowledge from different scientific fields as a key to advance our understanding of the Earth system (Clayson *et al.*, 2019).

Motivated by the urgency to fill this scientific knowledge gap, the main objective of this dissertation is to support different disciplines and research fields in need of meticulous information on terrestrial evaporation at different spatio-temporal scales by providing accurate satellite-based and observational data sets of terrestrial evaporation. In addition, the assets of these data sets are explored in two case studies within the fields of hydro-climatology and climate reanalysis, thereby showing the versatility of the former to the scientific community and gaining insights on the global-scale variability of terrestrial evaporation and the quality of the turbulent fluxes in climate reanalyses. More specifically, the three key objectives of this dissertation are formulated as:

1. To support global hydrological, atmospheric, and climate studies by deriving a global data set of terrestrial evaporation from satellite data at coarse spatial resolution (i.e. ± 25 km).
2. To aid local water resources management and agricultural planning by deriving a pilot data set of terrestrial evaporation for The Netherlands, Flanders, and the west of Germany from satellite data at high spatial resolution (i.e. 100 m).
3. To reveal the potential of the global data set derived in this dissertation for benchmarking climate reanalyses and to advance our understanding of the global-scale variability of terrestrial evaporation.

These objectives are tackled in Chapters 2–6 and in their dedicated scientific publications. A more detailed motivation, specific objectives, and relevant literature are provided in the introductory sections of each chapter. Below, the structure of this dissertation is presented.

1.3 Structure of this dissertation

Figure 1.2 gives an overview of the objectives defined in Section 1.2 and the chapters they are tackled in. The first part of this dissertation (Chapters 2 and 3) targets the first objective defined in Section 1.2 and focuses on the

advancement of GLEAM to derive global-scale data sets of terrestrial evaporation. More specifically, Chapter 2 elaborates on the potential of satellite-based surface soil moisture to improve estimates of terrestrial evaporation via data assimilation, a technique aiming to combine observations and model estimates of soil moisture in an optimal way (based on their relative uncertainties) to obtain a superior estimate of soil moisture (Martens *et al.*, 2016). Chapter 3 builds upon Chapter 2 by further refining the data assimilation system in GLEAM and improving various other model components aiming at a better representation of the land surface constraint on terrestrial evaporation (Martens *et al.*, 2017). In Chapter 3, a comprehensive global-scale validation of terrestrial evaporation and root-zone soil moisture derived using GLEAM is also presented.

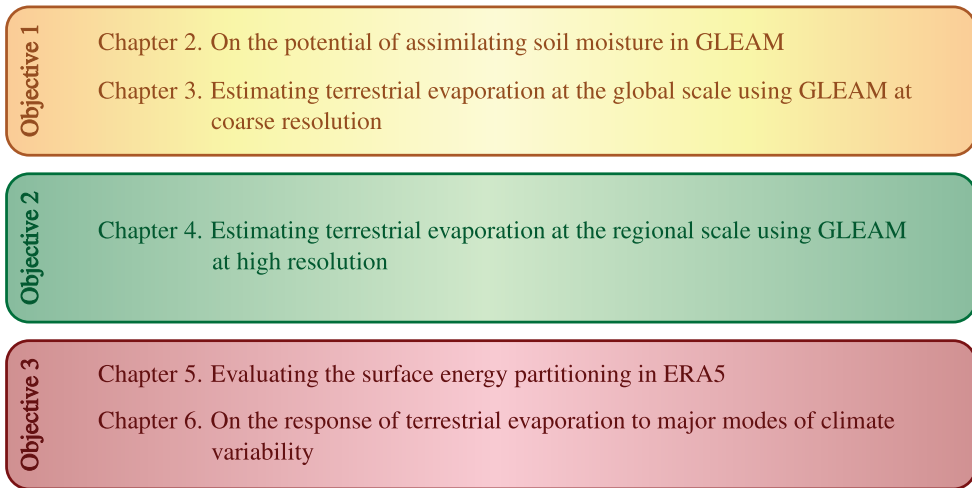


Figure 1.2: Overview of the chapters of this dissertation and their associated objectives.

The second part of this dissertation (Chapter 4) aims to meet the second objective defined in Section 1.2 and assesses the potential of GLEAM to be applied at high resolution and to derive root-zone soil moisture and terrestrial evaporation at scales useful for local water management and agricultural planning (Martens *et al.*, 2018a). In this chapter, a pilot data set for The Netherlands, Flanders, and the west of Germany at 100 m spatial and daily temporal resolution is also presented, and it is validated using in situ measurements of surface soil moisture and terrestrial evaporation.

The third part of this dissertation (Chapters 5 and 6) tackles the last objective defined in Section 1.2 and presents two case studies where the assets of GLEAM for (1) benchmarking climate reanalyses and (2) advancing our knowledge of the global-scale variability of terrestrial evaporation are shown. In particular, in Chapter 5, the quality of terrestrial evaporation –

and surface energy partitioning in general – in ERA5, a climate reanalysis from the European Centre for Medium-Range Weather Forecasts (ECMWF), is assessed and compared to its predecessor ERA-Interim (Martens *et al.*, 2019). The analysis is (among others) based on the use of a data set derived using GLEAM (Chapter 3) as a tool to evaluate the land surface modelling scheme in the reanalysis framework. Chapter 6 presents the results of a study analysing the impact of internal climate variability – induced by patterns such as the El Niño Southern Oscillation (ENSO) – on the dynamics of terrestrial evaporation (Martens *et al.*, 2018b), thereby providing insights on the global-scale and multi-decadal variability of terrestrial evaporation.

Finally, Chapter 7 summarises the most important conclusions of this dissertation, lists the main limitations, and presents a path forward to further advance GLEAM and to steer research on the monitoring of terrestrial evaporation.

CHAPTER 2

On the potential of assimilating soil moisture in GLEAM

This chapter introduces the baseline description of GLEAM and explores the potential of surface soil moisture assimilation into the former to improve estimates of terrestrial evaporation and root-zone soil moisture over continental Australia. Satellite-based observations of surface soil moisture from the Soil Moisture and Ocean Salinity mission are assimilated using a Newtonian Nudging algorithm in a series of experiments. Model estimates of surface soil moisture and terrestrial evaporation are validated against in situ measurements, and analogous experiments in which soil moisture retrievals from the Advanced Microwave Scanning Radiometer for Earth are assimilated are also conducted. This chapter is an edited version of the following scientific publication:

Martens, B., Miralles, D.G., Lievens, H., Fernández-Prieto, D., Verhoest, N.E.C., 2016. Improving terrestrial evaporation estimates over continental Australia through assimilation of SMOS soil moisture. *International Journal of Applied Earth Observation and Geoinformation* 48 (6), 146–162.

2.1 Introduction

Since the beginning of the previous century, several techniques have been developed to measure terrestrial evaporation in the field (Section 1.1.3). Despite the impact of multiple error sources on these types of measurements, in situ observations usually provide a rather accurate estimate of terrestrial evaporation at a given point in space and time. Unfortunately, these measurements remain insufficient to provide a clear understanding of the variability of terrestrial evaporation over large spatial domains (e.g. continental to global scales) and multi-decadal periods. Given the relevance of these scales for hydrological, agricultural, and climatological applications, the need for more advanced techniques has emerged. Due to the shortcomings of in situ measurements, the value of remote sensing to retrieve estimates of terrestrial evaporation from space (Section 1.1.4) has been extensively explored over the last three decades (Zhang *et al.*, 2016a; Wang and Dickinson, 2012; Kalma *et al.*, 2008). Different international activities have focused on the advancement in the field of remote sensing and terrestrial evaporation, e.g. the NASA Energy and Water cycle Study (NEWS), the European Union WATer and global CHange project (WATCH), the Global Energy and Water-cycle EXperiment (GEWEX) LandFlux initiative, or ESA's WATer Cycle Multimission Observation Strategy (WACMOS) project. Given the fact that terrestrial evaporation cannot be directly sensed from space, mathematical models that combine satellite-observable variables that are linked to the process of evaporation (e.g. radiation, temperature, soil moisture), are usually applied to derive estimates of terrestrial evaporation at the continental scale (Sections 1.1.2 and 1.1.4). The continuous development of satellite sensors and computing science allows the improvement of these existing models and facilitates the development of new ones.

The majority of process-based models dedicated to the retrieval of terrestrial evaporation from satellite data aim first at the accurate estimation of potential evaporation, using observations of meteorological variables like radiation, air temperature, air humidity, or wind speed. Estimates of potential evaporation are subsequently converted into actual terrestrial evaporation using different (empirical) factors that account for evaporative stress (i.e. the land surface constraint over the atmospheric demand for water). Existing models disagree to a large extent in their formulation of this stress, which in nature depends on soil-water content, vegetation physiology, and several phenological constraints. Most of these models do not directly consider the availability of water in the root zone, a major constraint on terrestrial evaporation, particularly in water-limited regions (Vinukollu *et al.*, 2011; Ferguson and Wood, 2010). As an exception, GLEAM (Miralles *et al.*, 2011b) constrains the atmospheric demand for water using microwave observations of precipitation, soil moisture, and vegetation optical depth (VOD). The latter is used as a proxy for the vegetation water content (Liu *et al.*, 2013). GLEAM can benefit from advances in any of

the satellite observations used in the model, including surface soil moisture. In this sense, ESA's Soil Moisture and Ocean Salinity (SMOS) mission (Kerr *et al.*, 2001) provides an opportunity to improve the data sets of terrestrial evaporation derived using GLEAM. SMOS is the first polar-orbiting, two-dimensional, interferometric L-band radiometer fully dedicated to the retrieval of surface soil moisture and ocean salinity. Since its launch in 2009, it provides global maps of brightness temperatures and higher-level geophysical products (e.g. surface soil moisture, VOD, and surface roughness) at a nominal spatial resolution of 43 km and revisiting times of approximately 3 days. Initially, research regarding the SMOS soil moisture products has mainly focused on the development and optimisation of retrieval algorithms (e.g. Martens *et al.*, 2015; Kerr *et al.*, 2012; Escorihuela *et al.*, 2007; Saleh *et al.*, 2007; Wigneron *et al.*, 2007; Pardé *et al.*, 2004) and on the validation of these retrievals using data from in situ networks (e.g. Su *et al.*, 2013; Al Bitar *et al.*, 2012; Jackson *et al.*, 2012) or other satellite-derived and modelled data sets of soil moisture (e.g. Leroux *et al.*, 2013). Later, studies started to investigate the value of SMOS soil moisture to improve model simulations of different hydrological variables (e.g. Lievens *et al.*, 2016, 2015; Dumedah and Walker, 2014b,a; Ridler *et al.*, 2014; Wanders *et al.*, 2014). Such studies are valuable means to investigate the potential of SMOS for integrated water management, and provide an alternative way to validate SMOS observations that is complementary to traditional comparisons to in situ data.

Given the potential value of surface soil moisture retrieved from SMOS for evaporation modelling, the main objectives of this chapter are to investigate the added value of the geophysical retrievals from SMOS to reduce uncertainty in the estimates of terrestrial evaporation and root-zone soil moisture from GLEAM, and to explore how SMOS soil moisture can be optimally integrated in GLEAM. In addition, this chapter also introduces the baseline description of GLEAM which serves as a reference for Chapters 3–6. To investigate the value of SMOS for GLEAM, several data assimilation experiments using a simple Newtonian Nudging algorithm are conducted over continental Australia. Data assimilation aims to optimally combine modelled and observed soil moisture (based on their relative uncertainties) to retrieve a superior estimate of the variable, and is thus a promising tool to improve the estimates of root-zone soil moisture and terrestrial evaporation in GLEAM. The model simulations in the different experiments are validated against in situ measurements of surface soil moisture and terrestrial evaporation over Australia. The results obtained by assimilating SMOS soil moisture are also compared to similar experiments using soil moisture from the Advanced Microwave Scanning Radiometer for Earth (AMSR-E). The chapter is organised as follows: Section 2.2 describes GLEAM and the data assimilation system used in this chapter. Section 2.3 gives an overview of the data sets used to force GLEAM and the in situ data

used to validate the modelled evaporation and soil moisture. In Section 2.5 the results of this chapter are presented, and in Section 2.6 a summary of the main findings is provided.

2.2 Methodology

2.2.1 Baseline description of GLEAM

GLEAM is a set of algorithms separately estimating the different components of terrestrial evaporation, i.e. transpiration, bare soil evaporation, open-water evaporation, interception loss, and sublimation (Section 1.1.1). The model aims at combining satellite retrievals linked to the physical process of evaporation and was originally developed to run at the global scale and daily resolution (Miralles *et al.*, 2011b). The model is typically applied on a spatially discrete grid where each grid cell comprises up to four different land cover types: bare soil, low vegetation (e.g. grasslands), tall vegetation (e.g. trees), and open water (e.g. lakes). Grid cells can also be covered by snow, in which case the entire evaporative flux is composed of sublimation (i.e. no transpiration, nor bare soil or open water evaporation). The evaporative flux is calculated for each of these fractions separately and then aggregated to the scale of the grid cell based on the fractional cover of each land cover type. Figure 2.1 shows a schematic overview of GLEAM and its modules, and a list of forcing variables is given in Table 2.1. A detailed description of the model version used in this chapter (GLEAM v2) is provided in Miralles *et al.* (2014), Miralles *et al.* (2011b), and Miralles *et al.* (2010), with the essential information for this chapter summarised below.

The model consists out of four components: the evaporation module, the stress module, the soil-water balance module, and the rainfall interception model (Figure 2.1). The evaporation module is used to calculate potential terrestrial evaporation using the Priestley and Taylor equation (Priestley and Taylor, 1972), which is preferred over the more complete Penman-Monteith equation (Monteith, 1965) because of its simplicity (Section 1.1.2). Hence, the model does not rely on variables which are difficult to observe from space (i.e. wind speed) or for which only short temporal records exist at the required resolutions (e.g. air humidity). The Priestley and Taylor equation calculates potential terrestrial evaporation based on net radiation and air temperature as:

$$\lambda \rho E_p = \alpha \frac{\Delta}{\Delta + \psi} (R_n - G), \quad (2.1)$$

where E_p is potential terrestrial evaporation ($\text{m}\cdot\text{s}^{-1}$), α is the Priestley and Taylor coefficient ($-$), Δ is the slope of the saturated water vapour-temperature curve ($\text{Pa}\cdot\text{K}^{-1}$), and ψ is the psychrometric constant ($\text{Pa}\cdot\text{K}^{-1}$). Both λ and Δ are functions of air temperature and are empirically estimated using the

equations provided by Henderson-Sellers (1984) and Maidment (1993), respectively. As remotely-sensed observations of G are not available, G is estimated as a constant fraction of R_n in GLEAM depending on the land cover type as described in Miralles *et al.* (2011b). For α , a value of 1.26 has been reported by Priestley and Taylor (1972) for well-watered grasslands, and has been used in numerous studies for a variety of ecosystems, including GLEAM where this default value is used for the fractions of bare soil, short vegetation, and open water. However, empirical studies have highlighted the more conservative nature of tree stomata, often resulting in lower rates of potential evaporation in forested areas (Teuling *et al.*, 2010; Kelliher *et al.*, 1993; Shuttleworth and Calder, 1979). Therefore, the α for tall vegetation is defined after the experimental findings by Eaton *et al.* (2001), Diawara *et al.* (1991), Viswanadham *et al.* (1991), Shuttleworth *et al.* (1984), and McNaughton and Black (1973), that report an average value of 0.97 (with a 0.08 standard deviation over the different studies) for various forests during unstressed and precipitation-free periods (i.e. no rainfall interception). For snow-covered grid cells, sublimation is calculated using a specific parameterisation of the Priestley and Taylor equation described in Murphy and Koop (2005)¹.

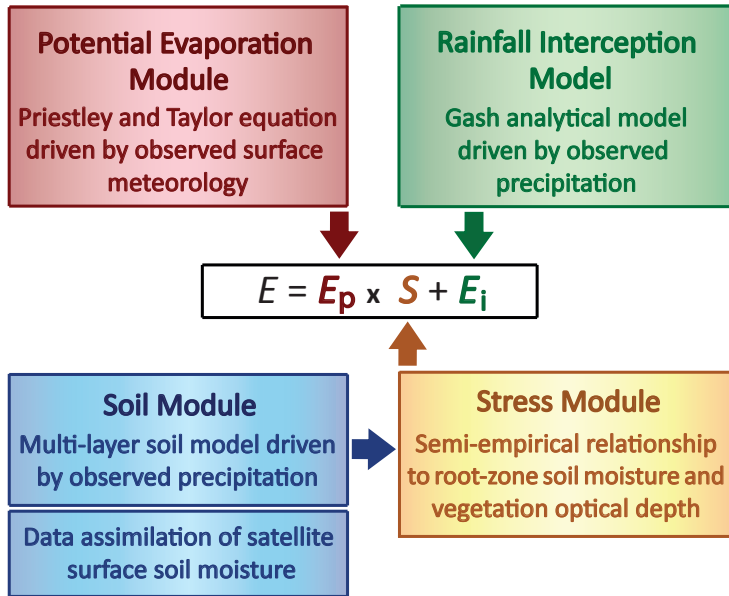


Figure 2.1: Schematic representation of GLEAM and its four modules. Note that the equation shown in the center is a simplified version of the one actually implemented in GLEAM (Equation 2.3), not considering the reduction in transpiration during rainfall interception loss.

¹Note that snow is not considered in this chapter; hence no snow product is listed in Table 2.1.

For each land cover fraction per grid cell, E_p is converted into actual terrestrial evaporation using an empirical, multiplicative stress factor, ranging from a value of one (no stress) to zero (maximum stress). This stress factor is parameterised in GLEAM v2 as a function of VOD, a proxy of vegetation water content (Liu *et al.*, 2013), and root-zone soil moisture:

$$S = [1 - (\vartheta_{\max} - \vartheta)] \frac{w^{(w)} - w_{\text{wp}}}{w_c - w_{\text{wp}}}, \quad (2.2)$$

where S is the evaporative stress factor (-), $\vartheta_{\max}$ is the annual maximum VOD (-), ϑ is the VOD (-), $w^{(w)}$ is the soil moisture content of the wettest model layer ($\text{m}^3 \cdot \text{m}^{-3}$), w_{wp} is the wilting point ($\text{m}^3 \cdot \text{m}^{-3}$), and w_c is the critical soil moisture ($\text{m}^3 \cdot \text{m}^{-3}$). For the fraction of bare soil, S is defined by the soil moisture alone (i.e. no impact of VOD), while for the open-water fraction S is set to one (i.e. no evaporative stress). Assuming that vegetation is able to extract water from soil layers from which water is more easily available, $w^{(w)}$ represents the soil moisture from the wettest layer of the soil-water module (module described below). The rationale of the stress function is that for soil moisture values between w_{wp} and w_c , the stress is linearly decreasing following a slope that is set by the VOD (Miralles *et al.*, 2014). Outside these boundaries, there is either maximum stress ($w \leq w_{\text{wp}}$) or no stress ($w \geq w_c$). The VOD is used to capture the effects that seasonal phenological changes (e.g. harvesting, leaf-out) or sudden vegetation declines (e.g. forest fires, clear cuts) have on transpiration.

The soil-water module in GLEAM calculates the root-zone soil moisture using a simple water-balance algorithm considering surface inputs (i.e. precipitation minus interception loss plus snowmelt) and outputs (transpiration, bare soil evaporation, and drainage). The number of soil layers is cover-dependent: three vertical soil layers for the tall vegetation fraction (0–10 cm, 10–100 cm, and 100–250 cm) and two layers for the short vegetation fraction (0–10 cm and 10–100 cm). For the bare soil fraction, it is assumed that only the first layer of soil (0–10 cm) contributes to the evaporative flux. Drainage fluxes between each pair of layers, and out of the soil profile, are simply calculated as the excess volume of water with respect to field capacity. Hence, for each model time step, it is assumed that all soil layers drain to field capacity (Miralles *et al.*, 2011b).

The last module calculates the rainfall interception loss – the direct vaporisation of intercepted rain by vegetation – for the tall vegetation fraction using the analytical model introduced by Gash (1979) and further refined by Valente *et al.* (1997). The basic assumptions of the Gash model are that there is only one storm per model time step and that the canopy dries out completely in between rainfall events. Note that, therefore, interception loss is only calculated for the fraction of tall vegetation in GLEAM as due to the relatively low aerodynamic

roughness of lower vegetation types, resulting in low evaporation rates during rainfall, their canopy may remain wet in between storms (Miralles *et al.*, 2010). However, the fraction of total evaporation originating from interception loss in these low vegetation types is relatively low as compared to forests, making it less important to model this process separately (Miralles *et al.*, 2010). In essence, the Gash model identifies three phases during each storm: wetting up of the canopy, saturated canopy, and drying out after the rainfall event. Water can be stored in both canopy and trunks, and the maximum storage capacity of both is parameterised based on values found in literature (Miralles *et al.*, 2010). For each phase during the event, the amount of water stored in the canopy is calculated as the balance between incoming rainfall - i.e. the fraction of rain that hits the canopy (parameterised using the fraction of tall canopy) - evaporation, and stem flow (after saturation of the canopy occurs, i.e. during the second phase). The rates of evaporation from the wet vegetation - originating from both the canopy and trunks - and incoming rainfall are both assumed to be constant during each event. While a constant evaporation rate is applied for all events as described in Miralles *et al.* (2010), the rainfall rate is estimated for each event separately as a linear function of the lightning frequency. The latter is based on the fact that substantially different intensities are typically found between frontal and convective rain, and that lightning only occurs during convective events. The Gash model implemented in GLEAM thus considers both the characteristics of precipitation and vegetation to model rainfall interception loss for the fraction of tall canopy (Miralles *et al.*, 2010). Note that, despite the fact that the model is not calibrated but parameterised based on values found in literature, it has been extensively validated against in situ data in Miralles *et al.* (2010), and has proven to perform well.

The final estimate of terrestrial evaporation in GLEAM for a specific land cover fraction in the grid cell is calculated as:

$$E = SE_p + E_i - \kappa E_i, \quad (2.3)$$

where E_i is the interception loss ($\text{m}\cdot\text{s}^{-1}$) modelled using Gash's analytical model and κ is a constant set to 0.07, which corrects for the reduction in transpiration when the canopy is wet and interception loss occurs (Gash and Stewart, 1977). Note again that interception loss in GLEAM is only calculated for the fraction of tall vegetation in the grid cell (i.e. $E_i = 0$ for the other land cover fractions), and that the total flux for the grid cell is obtained by calculating the average of the cover-dependent terrestrial evaporation, using the fractional cover in the grid cell as weights.

2.2.2 Data assimilation framework

Newtonian Nudging

To correct for the effects of random forcing errors, errors in the ancillary data (e.g. soil parameters), and uncertainties that are introduced by the choice of a simple bucket model in GLEAM, satellite soil moisture can be assimilated into the soil profile of GLEAM (Miralles *et al.*, 2014, 2011b). Here, a Newtonian Nudging scheme (Houser *et al.*, 1998) is implemented in GLEAM to update the modelled soil moisture states using remotely-sensed surface soil moisture observations. Newtonian Nudging is a simple assimilation technique that nudges the model states towards the soil moisture observations using the following equation:

$$\hat{w}^{(l)+} = \hat{w}^{(l)-} + K \frac{\sum_{i=1}^N W_i^2 \gamma_i (w_i^o - \hat{w}_i^-)}{\sum_{i=1}^N W_i}, \quad (2.4)$$

where $\hat{w}^{(l)+}$ is the a posteriori soil moisture state ($\text{m}^3 \cdot \text{m}^{-3}$) at layer l (i.e. the state after application of the assimilation algorithm), $\hat{w}^{(l)-}$ is the a priori soil moisture state ($\text{m}^3 \cdot \text{m}^{-3}$) at the same layer (i.e. prior to the assimilation step), w_i^o is the i^{th} observation of soil moisture ($\text{m}^3 \cdot \text{m}^{-3}$) out of N to be assimilated, $\hat{w}_i^-$ is the corresponding model estimate ($\text{m}^3 \cdot \text{m}^{-3}$), K is the nudging factor ($-$), W_i is the interpolation weight ($-$) given to observation i , and γ_i is the quality factor ($-$) for observation i .

Essentially, Equation 2.4 calculates a weighted average of model innovations (i.e. the difference between a certain observation and its corresponding a priori model state: $w_i^o - \hat{w}_i^-$) and uses this to update the a priori soil moisture state of interest. Hence, observations that do not directly correspond to the state of interest (e.g. observations taken at a certain distance in space or time) can still be used to update the latter by taking properly into account the dependency between the two via the interpolation weight W_i . The number of observations (N) used to update the soil moisture state at layer l depends on the radius of influence (i.e. whether the observations somehow relate to the state of interest) of these observations (Houser *et al.*, 1998). The interpolation weights (W_i) should thus be expressed based on the dependence between the soil moisture state of interest and the observation used to update this state. If there is a high dependency between these two variables, a higher interpolation weight should be attributed to this observation. Observations at different locations (horizontally and/or vertically) and different time steps can thus be used to update the state at a particular model time step and location. For this study, all model states at a given grid cell (i.e. at all three model layers) and time step, are exclusively updated using the observation coinciding with the

grid cell under consideration (i.e. no horizontal interpolation), and acquired within the model time step (i.e. no interpolation in time). Given the limited sensing depth of microwave sensors into the soil, which is often just a few centimetres depending on the soil wetness and sensing frequency (Schmugge, 1983), microwave soil moisture retrievals are considered to be representative of the first model layer here. Therefore, model innovations are only calculated for this layer. This innovation is subsequently used to update the model state at all three layers (vertical interpolation) using interpolation weights ($W^{(l)}$) equal to the long-term correlation between the modelled soil moisture at the first layer and the other layers. As a result, Equation 2.4 collapses to the following simpler form:

$$\hat{w}^{(l)+} = \hat{w}^{(l)-} + KW^{(l)}\gamma \left(w^o - \hat{w}^{(1)-} \right), \quad (2.5)$$

where w^o is the microwave-based soil moisture observation and $\hat{w}^{(1)-}$ is the corresponding a priori model state at layer 1. Here, K is set to one in order to ensure a maximum impact of the assimilation algorithm on the modelled soil moisture states.

Note that this simple assimilation algorithm uses a combination of a quality factor (γ) and a constant interpolation weight ($W^{(l)}$) to update the state variables at several model layers. Therefore, it misses several aspects of more complex data assimilation systems, such as those from the Kalman filter family, that account for the complex error-covariance structure between the different states and observations. However, using a simple assimilation algorithm, such as Newtonian Nudging, falls within the rationale of GLEAM to keep the method as simple and observation-driven as possible.

Estimation of the quality factor

The quality factor (γ) in Equation 2.5 is a parameter of the assimilation algorithm balancing model and observation errors. More specifically, γ is the weight attributed to the observation, while $(1 - \gamma)$ is the weight related to the a priori model state. γ should thus depend on both model and observation errors. If both errors are known, γ is calculated as follows:

$$\gamma = \frac{\sigma_{\text{mod}}}{\sigma_{\text{mod}} + \sigma_{\text{obs}}}, \quad (2.6)$$

where σ_{mod} and σ_{obs} are the standard deviations of the distribution of random model and observation errors ($\text{m}^3 \cdot \text{m}^{-3}$), respectively. To objectively estimate both parameters, a Triple Collocation Analysis (TCA; Miralles *et al.*, 2010; Scipal *et al.*, 2008; Stoffelen, 1998) is performed prior to the application of the data assimilation using the open-loop (OL) surface soil moisture from GLEAM, the satellite-based soil moisture observations that are assimilated,

and a third independent data set of surface soil moisture (Section 2.3.1). TCA is a statistical method to estimate the relative errors in three or more mutually independent data sets of the same geophysical variable. The assumption of independence is a prerequisite to obtain bias-free estimates of the errors (Yilmaz and Crow, 2014). In addition, TCA needs all three data sets to be pre-scaled into a common reference to account for potential biases (see further).

The TCA yields a temporally constant estimate of the error for each grid cell in the considered domain, and thus a γ that is constant in time as well (yet not in space). However, it is generally accepted that the accuracy of soil moisture retrieved from satellite observations is impacted by (among others) vegetation characteristics (Leroux *et al.*, 2013; Parinussa *et al.*, 2011; de Jeu *et al.*, 2008), with increasing vegetation density resulting in a reduced emissivity of the soil surface relative to the vegetation emissivity (de Jeu *et al.*, 2008). This implies that the soil moisture retrieval error varies in time as well, and that it is positively correlated to the vegetation density. Similarly, the error on the modelled soil moisture can also change in time due to e.g. structural errors in the algorithms, poor model calibration and – more importantly – dynamic errors in forcing data. To investigate this non-stationarity, the use of a dynamic γ is also considered in the assimilation experiments.

de Jeu *et al.* (2008) found that the retrieval error of AMSR-E soil moisture could be empirically related to the VOD. Based on these experiments, the following equation to estimate the error of microwave soil moisture is used here:

$$\sigma_{\text{obs}} = 0.2\vartheta^3 + 0.04 \quad (2.7)$$

This equation is in principle only valid for AMSR-E soil moisture observations and the corresponding VOD estimates based on the Land Parameter Retrieval Model (LPRM). However, given the similarities between SMOS and AMSR-E, it is assumed here that the retrieval accuracy of SMOS is equally impacted in time by VOD dynamics. Nonetheless, the VOD retrieved from SMOS needs to be bias-corrected to the AMSR-E VOD prior to its application in Equation 2.7 due to the different sensing frequency of SMOS (1.43 GHz) and AMSR-E (6.9 GHz) and thus their different sensitivities to vegetation properties. To this end, a classical Cumulative Distribution Function (CDF) matching approach is used (Reichle and Koster, 2004). After the calculations of σ_{obs} via Equation 2.7, the resulting error time series are re-scaled per grid cell by matching their temporal average to the static error estimated from the TCA. This yields an observation error with a different long-term mean for SMOS and AMSR-E, but with the same temporal dynamics, as only SMOS VOD is used in Equation 2.7 (for SMOS and AMSR-E) to be able to attribute the differences between the assimilation of SMOS and AMSR-E soil moisture to the change in soil moisture product only.

The dynamics of the model error are traditionally analysed by running a model ensemble with perturbed parameter values and forcing data. Here, the model error is characterised by generating an ensemble of 32 members as in Reichle and Koster (2004). The generation of the ensemble members was performed by perturbing the wilting point, the field capacity, and the rainfall fields. The soil parameters were perturbed with a multiplicative factor randomly generated from a normal distribution with unity mean and 0.1 standard deviation. The rainfall forcing was sampled around the measured value considering a normal distribution with standard deviation equal to the dynamic rainfall error (Huffman, 1997). Note that this type of perturbation can lead to negative values, which were avoided by repeating the perturbation if negative values were generated. To be consistent with the characterisation of the observation errors (described above), the long-term average of the resulting dynamic errors for soil moisture at each grid cell is rescaled to match the static model error obtained using the TCA. Equation 2.7 and the model ensemble are thus only used to retrieve the dynamics of the observation and model errors, respectively, while the long-term average value of the errors is determined by TCA as in the case of a constant γ .

Rescaling of observations

A major challenge with regard to the assimilation of observed states into land surface models is the potential existence of a systematic mismatch between modelled and observed states (Verhoest *et al.*, 2015; Kumar *et al.*, 2012; De Lannoy *et al.*, 2007; Reichle and Koster, 2004). Mismatches in soil moisture states result from differences in horizontal and vertical scales between products (Sahoo *et al.*, 2013; Wilker *et al.*, 2006), simplifications in both the land surface model and the soil moisture retrieval algorithm (De Lannoy *et al.*, 2007), and errors in forcing and ancillary data sets such as soil parameters. Because of this mismatch, even if soil moisture products show similar dynamics, the range and absolute values may differ. However, data assimilation approaches generally require a common range for the modelled and observed soil moisture states. As a result, several studies have tried to define a straightforward way to deal with these systematic differences. To date, there is no consensus in literature and the choice of the scaling method remains ultimately subjective (Lievens *et al.*, 2015). For this study, observations are scaled to the open-loop simulations (no data assimilation) at each grid cell prior to the data assimilation. A classical CDF-matching approach (Reichle and Koster, 2004) is used here, which accounts for all moments of the distribution and ensures that the range of soil moisture observations equals the range of modelled states. Since the CDF-matching is based on the entire multi-year time series, the scaling does not remove shorter-scale variability differences, like seasonal biases or multi-day anomalies. Note that these CDF-matched soil moisture data sets can be

directly used in the TCA as well to estimate the errors.

2.3 Data

2.3.1 Input data sets

An overview of the different input data sets used in this study can be found in Table 2.1. Data are processed for continental Australia at a temporal resolution of 6 hours, and on a grid with a spatial resolution of 0.25° . Data available at different native spatial resolutions are linearly resampled on the defined grid and a similar approach is used to disaggregate the time series to the required temporal resolution, if needed. Note that more details on the experimental setup are given in Section 2.4.

Table 2.1: List of the selected forcing data sets together with an indication of the type of data, their approximate native spatial and temporal resolution, and their reference.

Variable	Data set	Type	Resolution		References
			Spatial	Temporal	
Radiation	CERES L3 SYN1DEG Ed4A	Satellite	110 km	3 hours	Doeling (2017)
Precipitation	TRMM 3B42 v7	Merge	27 km	3 hours	NASA GES DISC (2018)
Temperature	ERA-I	Reanalysis	80 km	6 hours	Dee <i>et al.</i> (2011)
VOID	SMOS LPRM	Satellite	27 km	3 days	van der Schalie <i>et al.</i> (2015b,a)
Soil moisture	SMOS L3	Satellite	25 km	3 days	Jacquette <i>et al.</i> (2010)
	AMSR-E LPRM L3 v001	Satellite	27 km	2 days	de Jeu and Owe (2013)
	MERRA-Land	Reanalysis	74 x 55 km	1 hour	Reichle <i>et al.</i> (2011)
Cover fractions	MOD44B v051	Satellite	27 km	1 year	Dimiceli <i>et al.</i> (2015b)
Soil properties	IGBP-DIS	Survey	27 km	static	Global Soil Data Task Group (2000)
Lightning	LIS/OTD	Satellite	5 km	1 month	Cecil <i>et al.</i> (2014)

Dynamic forcing data are preferentially derived from satellite observations. An exception is the near-surface air temperature product sourced from ECMW's Reanalysis (ERA)-Interim (Dee *et al.*, 2011), hereafter referred to as ERA-I. This product was chosen because 6-hourly satellite-based products of (all-skies) air temperature are not available. Observations of surface net radiation (CERES L3 SYN1DEG Ed4A; Doeling, 2017) are based on measurements from the Clouds and Earth's Radiant Energy System (CERES; Wielicki, 1996) onboard Terra and Aqua, while precipitation comes from the Tropical Rainfall Measuring Mission (TRMM) 3B42 v7 product (NASA GES DISC, 2018; Huffman *et al.*, 2007). The reported root mean square errors from 3B42 v7 (Huffman, 1997) are also used in the ensemble generation experiment described in Section 2.2.2. Finally, the VOD is retrieved from SMOS observations using the LPRM (van der Schalie *et al.*, 2015b,a; Owe *et al.*, 2008). Given that VOD is a forcing variable in GLEAM, it needs to be gap-filled; this is done using a local regression smoother with a window of one month, which also allows the removal of short-scale, unrealistic fluctuations in the time series. Note that snow sublimation is not considered in this chapter, hence Table 2.1 does not list any data set to monitor this variable.

Microwave soil moisture retrievals from SMOS (Kerr *et al.*, 2001) and AMSR-E (Kawanishi *et al.*, 2003) are also collected and processed for continental Australia. SMOS Level 3 data from the Centre Aval de Traitement des Données (CATDS; Jacquette *et al.*, 2010) are collected for the entire study period. These data are provided at an Equal Area Scalable Earth (EASE) grid with an approximate grid size of 25 km. For AMSR-E, the daily Level 3 LPRM soil moisture product (de Jeu and Owe, 2013) is chosen, which is provided at the same 0.25° grid of the GLEAM model and is only available for the period September 2010 – October 2011. For both SMOS and AMSR-E, data from ascending and descending overpasses are available separately. While AMSR-E measures the surface emissivity in the C-band (6.9 GHz), SMOS uses an L-band frequency of 1.43 GHz that is less sensitive to vegetation, aiding the retrieval of surface soil moisture (Kerr *et al.*, 2001). The soil moisture products have been filtered using flags for radio frequency interference, snow, frozen soils, standing or open water, and dense vegetation cover. In addition, outliers have been removed from the data sets prior to the analysis by removing data falling outside the following window, calculated for each data set and grid cell separately: $[q_{25} - 1.5(q_{75} - q_{25}); q_{75} + 1.5(q_{75} - q_{25})]$, where q_{75} and q_{25} are the 75% and 25% quantiles of the data set, respectively. Additionally, a third independent surface soil moisture data set is needed to perform the TCA to assess the errors in the microwave and modelled soil moisture during the data assimilation (Section 2.2.2). To this end, the Modern Era Retrospective-Analysis for Research (MERRA)-Land (Reichle *et al.*, 2011) is used. MERRA-Land data are generated using the offline version of the land surface model in

MERRA, forced with gauge-corrected precipitation data.

Static data sets used in GLEAM store information about soil properties, vegetation cover fractions, and the average rainfall climatology used in the interception loss model (Section 2.2.1). Soil parameters, such as the critical soil moisture, wilting point, and field capacity, are extracted from the Global Gridded Surfaces of Selected Soil Characteristics (Global Soil Data Task Group, 2000). The latter is derived by spatially interpolating a global data set of pedon records (Global Soil Data Task Group, 2000). The land cover fraction per grid cell is taken from the Global Vegetation Continuous Fields product (MOD44B), based on MODIS observations (Hansen *et al.*, 2005) and is available at 0.25° spatial resolution. The product provides per grid cell the fractional tree cover, non-tree cover, and bare soil used to prescribe the fractions of tall vegetation, low vegetation, and bare soil in GLEAM, respectively. MOD44B is based on a statistical regression tree trained on high-resolution imagery and phenological metrics such as light penetration to the ground (Hansen *et al.*, 2005) to derive global fields of fractional land cover. Finally, the rainfall climatologies used in the interception loss model are derived from the Combined Global Lightning Flash Rate Density monthly product from NASA (Mach *et al.*, 2007) – see also Miralles *et al.* (2010).

2.3.2 Validation data sets

For validation purposes, in situ measurements of surface soil moisture and terrestrial evaporation from the Australian and New Zealand Flux Research and Monitoring Network OzFlux (<http://www.ozflux.org.au/>; last visit: 18 November 2019) and the International Soil Moisture Network (ISMN; Dorigo *et al.*, 2013, 2011) are used². Figure 2.2 shows the locations of these in situ sites and Table A.1 (Appendix A) lists the eddy-covariance sites used, together with their FLUXNET ID, International Geosphere-Biosphere Programme (IGBP) land cover classification, and official reference. The only selection criteria for the in situ stations were that the percentage of gaps in the record covering the study period could not exceed 35%, that at least 100 data records after masking were available, and that soil moisture sensors were installed at a maximum depth of 10 cm below the surface (i.e. within the first soil layer of GLEAM). Measurements from the selected stations were quality-checked by removing outliers (the same procedure as for the microwave soil moisture is used; Section 2.3.1), and in situ soil moisture stations falling within the same 0.25° grid cell of the model were averaged to obtain a single representative time series

²The ISMN provides access to soil moisture measurements from a large number of local and regional measurement networks in a common data format. Hence, the data set contains measurements taken with different techniques ranging from cosmic ray neutron sensors to more traditional time domain reflectometry sensors. More information can be found at <https://ismn.geo.tuwien.ac.at/en/>; last visit: 18 November 2019.

for the entire grid cell. For the eddy-covariance measurements, periods of rain have been masked from the in situ time series as the measurement technique is less reliable when the sensors are wet (Mizutani *et al.*, 1997). Finally, all time series are aggregated from their native temporal resolution to 6-hourly aggregates, allowing no missing values within the aggregation window. After processing, measurements of surface soil moisture and terrestrial evaporation are available from 25 and 12 (corresponding to roughly 30 site years) in situ sites, respectively.

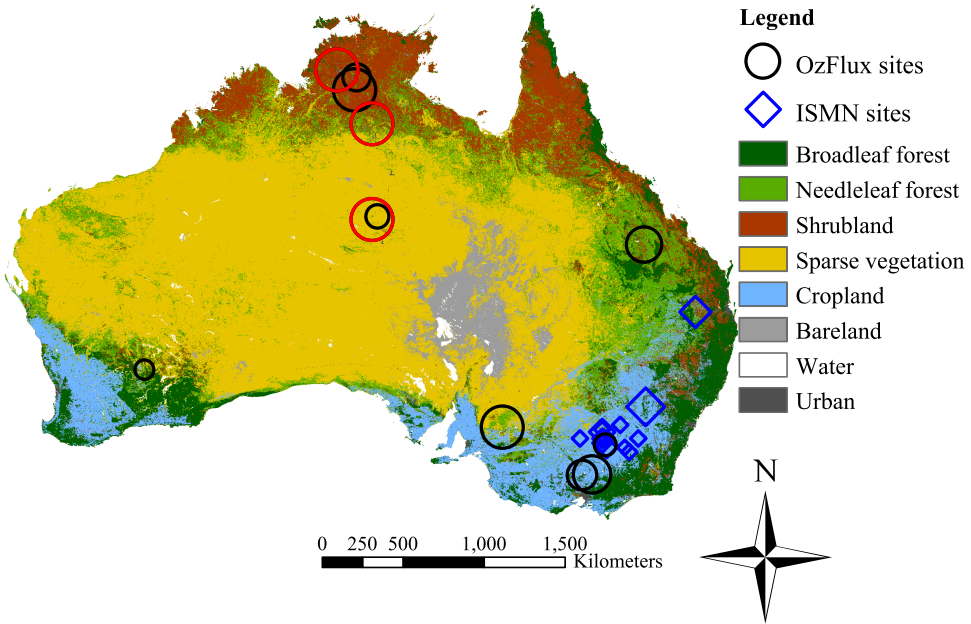


Figure 2.2: Land cover map (reclassification from GlobCover 2009) of continental Australia with indication of the in situ soil moisture sites (blue diamonds) and the eddy-covariance towers (black and red circles). The size of the symbols is directly proportional to the length of the data record at each site. Focus sites (i.e. sites reporting measurements of both soil moisture and terrestrial evaporation for the entire study period) are indicated using red circles.

Figure 2.2 shows that most ISMN sites are clustered in southeastern Australia (i.e. the Murrumbidgee catchment) and that the record length for these sites is generally lower than for other stations; yet the minimum length is approximately 250 days. OzFlux sites usually report a longer record, with five sites (AU-ASM, AU-Cpr, AU-DaS, AU-Dry, AU-Stp) spanning the entire validation period (1188 days) with measurements of soil moisture. Three of these sites (AU-ASM, AU-DaS, and AU-Stp) also report eddy-covariance measurements for the complete validation period. These sites will be used as focus sites in Section 2.5.3 and are indicated using red circles. Finally, Table A.1

(Appendix A) and Figure 2.2 indicate that most sites are dominated by short vegetation types such as grasslands, crops and/or shrubs.

2.4 Experimental setup

In this chapter, GLEAM is forced over continental Australia at a temporal resolution of 6 hours and on a grid with a spatial resolution of 0.25° . The 6-hourly temporal resolution allows for a more optimal assimilation of soil moisture observations than previous applications of the model at the daily scale, as the overpass time of the satellite and the model time step can be more closely matched (Miralles *et al.*, 2011b, 2014). Continental Australia comprises several climate zones and ecosystem types, resulting in strong seasonal, multi-annual, and spatial changes in terrestrial evaporation. Recently, it has been shown that the temporal dynamics of terrestrial evaporation in Australia strongly impact the multi-year variability of global evaporation (Miralles *et al.*, 2014; Jung *et al.*, 2010) and that the region can be considered as a hotspot of soil moisture–atmosphere interactions during summertime (Guillod *et al.*, 2014; Miralles *et al.*, 2012). The model is applied for the period 2010–2013 and the soil moisture of each model layer in GLEAM is initialised as the average of the wilting point and field capacity in the grid cell. The first eight months of the study period are used to spin up the model to remove the impact of the model initialisation, while the actual evaluation of the results is performed for the period September 2010–December 2013.

Several experiments are conducted with GLEAM to investigate the impact of different settings in the data assimilation system and to unravel the quality of different satellite-based data sets of surface soil moisture. First, TCA is used to assess the uncertainty in the data sets of surface soil moisture from GLEAM, SMOS, and AMSR-E (Section 2.3.1). In this analysis – next to investigating the quality of the combined ascending and descending data sets – the quality of both is also evaluated separately to investigate the impact of the satellite overpass time on the uncertainty of the retrieved soil moisture. Second, the use of a constant and dynamic γ in the proposed data assimilation framework (Section 2.2.2) is evaluated by assimilating SMOS surface soil moisture into GLEAM using both approaches. In addition, assimilation experiments are conducted using only ascending, descending, or both SMOS data sets to further unravel their quality differences. Next to the assimilation of SMOS soil moisture, surface soil moisture retrieved from AMSR-E is also assimilated into GLEAM to compare the quality of both satellite-based data sets. For each assimilation experiment, the corresponding OL simulation is used as a reference to analyse potential improvements upon a simulation without the assimilation of surface soil moisture. The impact of the data assimilation is assessed by evaluation of the estimated surface soil moisture (i.e. soil moisture

from the first model layer in GLEAM) and terrestrial evaporation at 6-hourly temporal resolution against in situ measurements (Section 2.3.2) using the Pearson correlation coefficient (R) and Root Mean Squared Difference (RMSD) as primary validation statistics. Finally, a time series analysis is performed at different focus sites (Section 2.3.2) and spatial patterns over continental Australia are visually analysed.

2.5 Results and discussion

2.5.1 Microwave soil moisture errors from TCA

Table 2.2 shows the average TCA errors for both SMOS and AMSR-E over the 25 soil moisture validation sites considered in this study. Three separate analyses were performed (Section 2.4): including only ascending data, only descending data, and a merger of the ascending and descending overpasses. A threshold of 100 triplets is used to ensure sufficient amount of data to perform the TCA (Scipal *et al.*, 2010). Note that for the GLEAM OL, the results from both the TCA with the triplet SMOS–GLEAM–MERRA-Land and AMSR-E–GLEAM–MERRA-Land are shown for comparison. Table 2.2 shows that, as expected, the TCA errors of GLEAM are on average the same for each experiment, regardless of the chosen triplet. Based only on this TCA, it can be concluded that (1) the OL soil moisture estimates of GLEAM are overall better than the satellite data sets, (2) the quality of the SMOS soil moisture retrievals is generally higher than that of AMSR-E, and (3) the ascending SMOS data set outperforms the descending SMOS data set, while the opposite happens in the case of AMSR-E (these results are also confirmed by the ground validations that will be presented in Section 2.5.2). The better performance of SMOS in the ascending overpass (6 am local solar time) is related to the fact that vegetation, air, and soil temperatures are approximately in equilibrium around that time (Jacquette *et al.*, 2013; Kerr *et al.*, 2011). The same is valid for the descending overpass of AMSR-E (1.30 am local solar time; Draper *et al.*, 2009; Njoku *et al.*, 2003). Since the radiative transfer models used to retrieve surface soil moisture make the assumption of no temperature gradient, the difference in quality between both overpasses can be strong, particularly for AMSR-E in which the ascending overpass occurs around noon (1.30 pm local solar time) when temperature gradients are typically higher (Draper *et al.*, 2009).

In Figure 2.3, the dynamic soil moisture errors of model and observations, together with the corresponding quality factor, are illustrated for an ISMN site in the Murrumbidgee catchment. Note that the time series shown for AMSR-E (Figure 2.3b) is shorter than the one for SMOS (Figure 2.3a) due to data availability (Section 2.3.1). Figure 2.3 shows that, for the overlapping period between SMOS and AMSR-E, the dynamic model error is approximately the same in both cases, but small differences may still occur from the use of a

Table 2.2: TCA errors ($\text{m}^3\cdot\text{m}^{-3}$) for SMOS, AMSR-E and the GLEAM open loop (OL). The statistics are reported for the ascending data only, descending data only, and the combined data set. Note that for the GLEAM OL, the results from both the TCA with the triplet SMOS–GLEAM–MERRA-Land and AMSR-E–GLEAM–MERRA-Land are shown for comparison. TCA errors obtained for MERRA-Land are not reported as they are beside the purpose of the study.

	Ascending	Descending	Ascending– Descending
SMOS	0.026	0.032	0.030
GLEAM OL	0.026	0.025	0.026
AMSR-E	0.036	0.024	0.033
GLEAM OL	0.025	0.024	0.025

different triplet in the TCA (Table 2.2). It can also be seen that the temporal variability of the observation error is the same for both SMOS and AMSR-E (which results from the common use of Equation 2.7 for both data sets), but the observation error for AMSR-E is on average higher due to the higher TCA error (Table 2.2). Figure 2.3 also illustrates the difference in dynamics between the smoothly varying estimates of the observation error (impacted by the VOD) and the highly variable model error (mainly impacted by rainfall events). Finally, it can be seen that the corresponding γ shows a higher average value for SMOS than for AMSR-E, as a result of the lower observation error (Table 2.2).

2.5.2 Validation of soil moisture

Surface soil moisture simulations from different assimilation experiments and the OL are validated against the in situ soil moisture measurements introduced in Section 2.3.2. Pearson correlation coefficients between the modelled and the measured soil moisture are calculated for the 25 in situ sites considered in this study. Figure 2.4 presents histograms of these correlation coefficients for the different assimilation experiments using a constant γ (Figures 2.4a) or a dynamic γ (Figures 2.4b), as well as assimilating SMOS ascending data, descending, or both. Blue represents the OL and red are the simulations with data assimilation, while purple indicates the overlap of both histograms. Overall, the average correlation coefficient of 0.68 for the OL (Figure 2.4) shows that there is a good agreement between modelled and in situ soil moisture. In addition, the assimilation of soil moisture is generally improving the OL results: when both the ascending and descending SMOS data are assimilated, the average correlation increases from 0.68 to 0.71, and a statistical significant (at the 5% significance level) increase in the correlations is achieved for 17 out of the 25 individual stations according to the Steiger test for paired correlations (Steiger, 1980). Based on the same statistical test, the assimilation

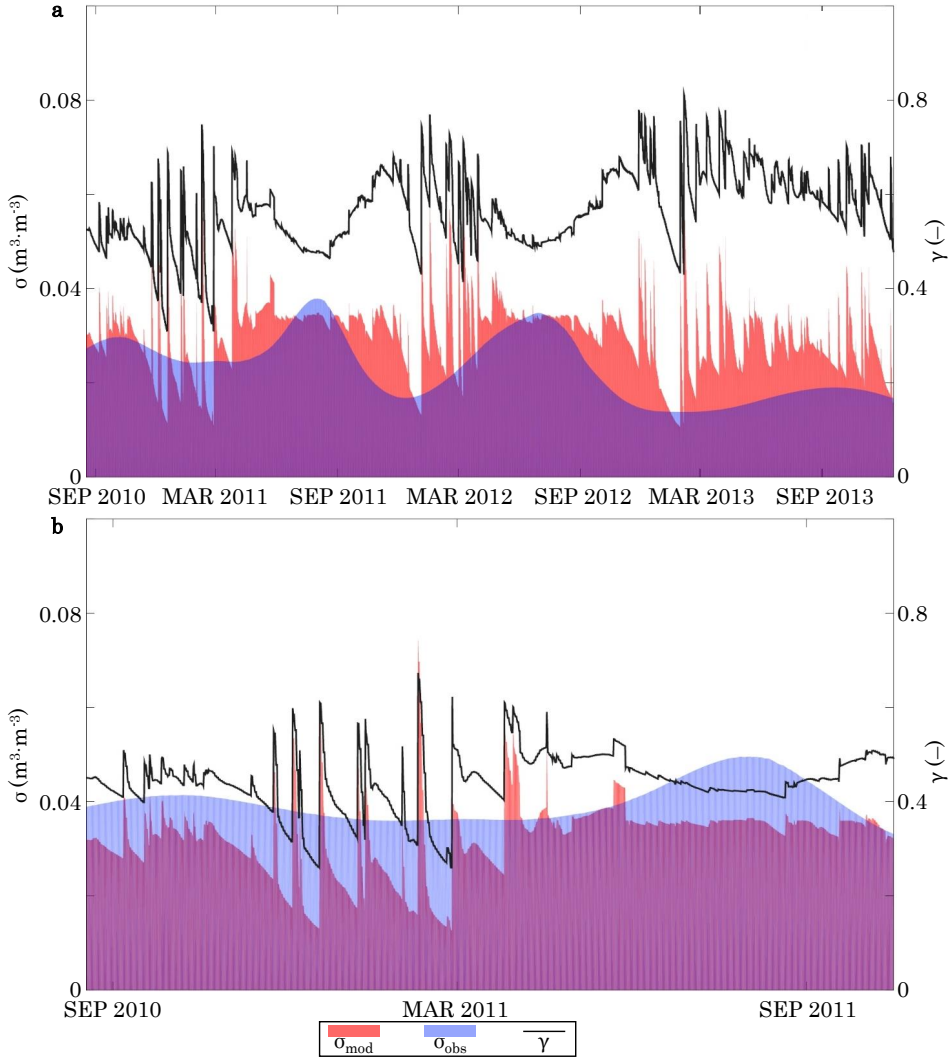


Figure 2.3: Time series of the model (σ_{mod}) and observation errors (σ_{obs}), and the corresponding quality factor (γ) at an ISMN site in the Murrumbidgee catchment for (a) SMOS and (b) AMSR-E. Note that the time series shown for AMSR-E is shorter than the one for SMOS due to data availability (Section 2.3.1).

of the ascending SMOS data set results in a significant increase of the correlation coefficients at 19 sites, while for the descending data set a significant increase is only achieved at 15 sites. These results indicate again the slightly lower quality of the descending SMOS data compared to the ascending data, as highlighted in Section 2.5.1. The results of the experiment with a dynamic quality factor (Figure 2.4b) point to the same conclusions, and indicate that

the consideration of a dynamic γ (as opposed to a constant one) yields very similar results here. Since GLEAM is developed to be applied at continental to global scales and it is built on the basis of simplicity, these findings are of importance, as using a constant γ circumvents the need to run ensembles and strongly reduces the computational demands. Therefore, unless otherwise noted, the remaining discussions and results in this chapter are based on the application of a constant γ in the assimilation framework.

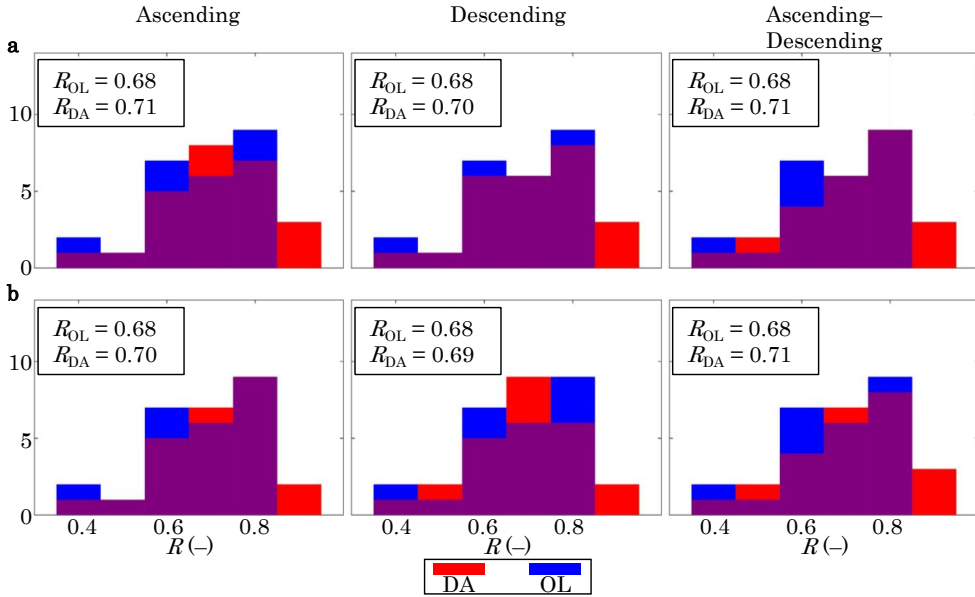


Figure 2.4: Histograms of the Pearson correlation coefficient (R) between the modelled and the in situ measured surface soil moisture at the 25 validation sites. Histograms for the open loop (OL) are shown in blue and for the simulations with data assimilation (DA) in red. Where both histograms overlap, a purple colour is used. Separate histograms are shown for the assimilation of only ascending data, descending data, and both ascending and descending data. The average correlation coefficient for all experiments is also reported. **(a)** Histograms for the experiment with a constant quality factor and **(b)** histograms for the experiment with a dynamic quality factor.

Figure 2.5 shows time series of modelled soil moisture for the complete study period for the focus sites AU-ASM (Figure 2.5a), AU-DaS (Figure 2.5b), and AU-Stp (Figure 2.5c) described in Section 2.3.2, together with the in situ measurements. For these figures, the combined ascending-descending SMOS data set was assimilated into GLEAM using a constant quality factor in the Newtonian Nudging scheme. For visual purposes only, all variables have been aggregated to daily intervals and the modelled soil moisture has been

CDF-matched against the in situ measurements. In Figure 2.5, the impact of the assimilation of surface soil moisture into GLEAM becomes more apparent, especially in periods with low rainfall, when soil moisture steadily decreases and evaporative stress rises (Peters-Lidard *et al.*, 2011). Figure 2.5 shows that these dry periods often occur in Austral winter, between March and September. In Figures 2.5b and c, it can be seen that in the dry period starting around March 2011, the assimilation tends to correct for the slow dry out in the model OL simulations, which is partly noticeable in the soil moisture time series. Conversely, the model estimates a steep dry out around March 2012 at AU-Stp that the assimilation algorithm is able to partly correct for. However, it can also be seen from Figure 2.5 that the assimilation of surface soil moisture into GLEAM often results in unrealistic high-frequency fluctuations in the modelled soil moisture that are not present in the in situ data. This can be explained by either noise in the observed signal from SMOS, the representativeness mismatch between the grid cell and the in situ soil moisture, or the sub-optimal configuration or simplicity of the data assimilation system.

2.5.3 Validation of terrestrial evaporation

Figure 2.6 shows Taylor plots (Taylor, 2001) of the validation statistics of the modelled evaporation at the 12 eddy-covariance sites for different experiments. Circles show the statistics for the OL, while the statistics for the simulations with assimilation of all SMOS data (i.e. ascending and descending observations) and a constant quality factor are plotted as squares. The different colours correspond to different validation sites. Following the procedure by Taylor (2001), both the centered RMSD and the standard deviation were normalised using the standard deviation of the observed time series such that the black diamonds in Figure 2.6 serve as a reference point for all other points.

Figure 2.6a shows the Taylor plots of the validation statistics of the modelled evaporation in the GLEAM OL and after assimilation of the combined SMOS ascending/descending data set (Pearson correlation coefficients against the in situ data at all sites for this experiment are listed in Table A.1; Appendix A). It can be seen that the model performs well in its OL with an average correlation coefficient of 0.75 over all stations, even if the modelled variability is larger than that of the observations at most eddy-covariance sites. This may in fact relate to errors in the in situ data, as several studies have already highlighted the lack of closure in the energy balance at several eddy-covariance sites and a consequent tendency to underestimate latent heat fluxes (Section 1.1.3). A common way to correct for the effects of this underestimation is to validate against the latent heat flux calculated as the residual from the energy balance at the eddy-covariance site (i.e. net radiation minus the ground heat flux and sensible heat flux) – see e.g. McCabe *et al.* (2016). Figure 2.6b shows that the overestimation of the variability in Figure 2.6a is strongly reduced when using

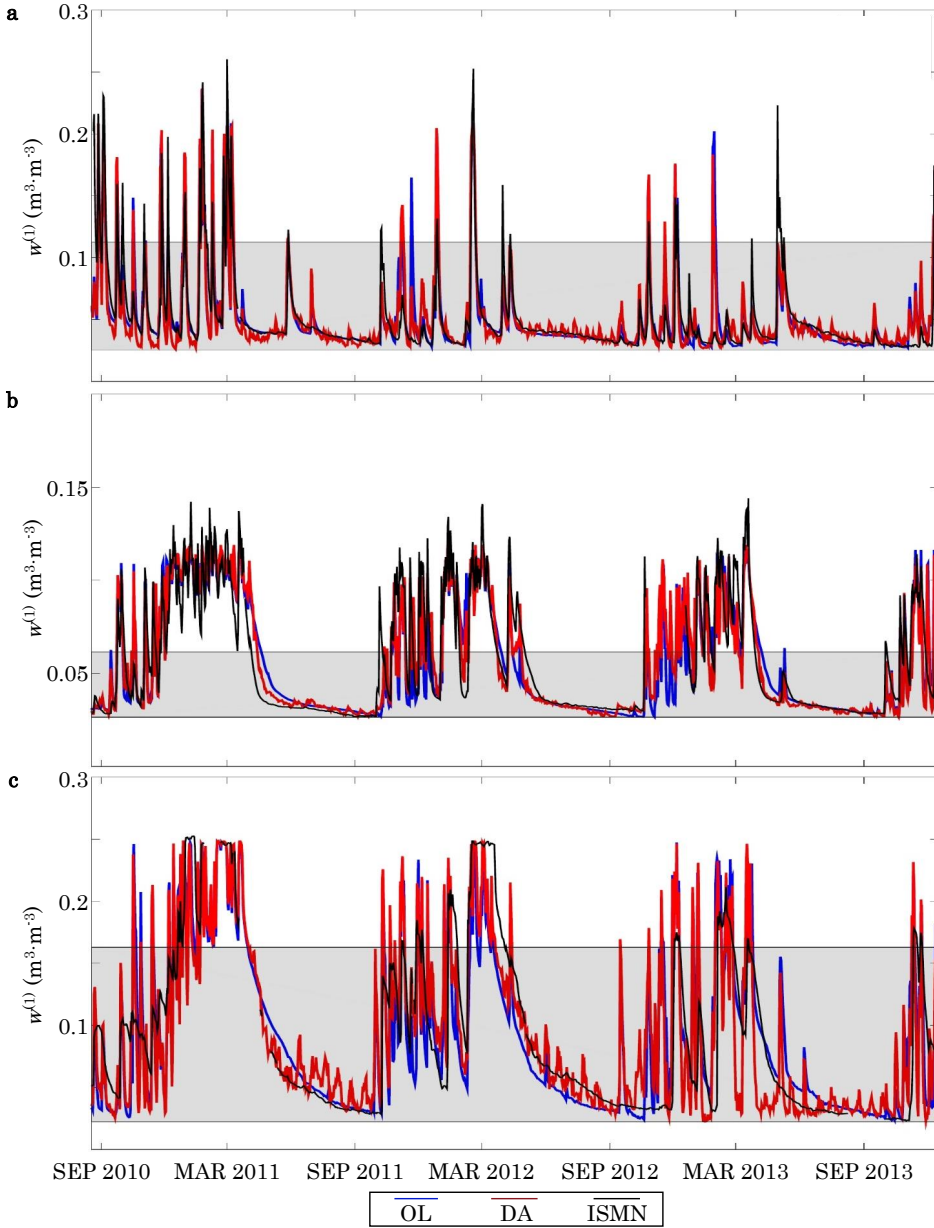


Figure 2.5: Time series of the modelled surface soil moisture ($w^{(1)}$). For this experiment, the complete SMOS data set is assimilated into GLEAM and a constant quality factor is used in the assimilation algorithm. The grey-shaded area in the figures shows the limits of the stress function (i.e. the critical soil moisture and wilting point). The simulations have been aggregated to daily scales for visual purposes. (a) Time series at site AU-ASM, (b) AU-DaS, and (c) AU-Stp.

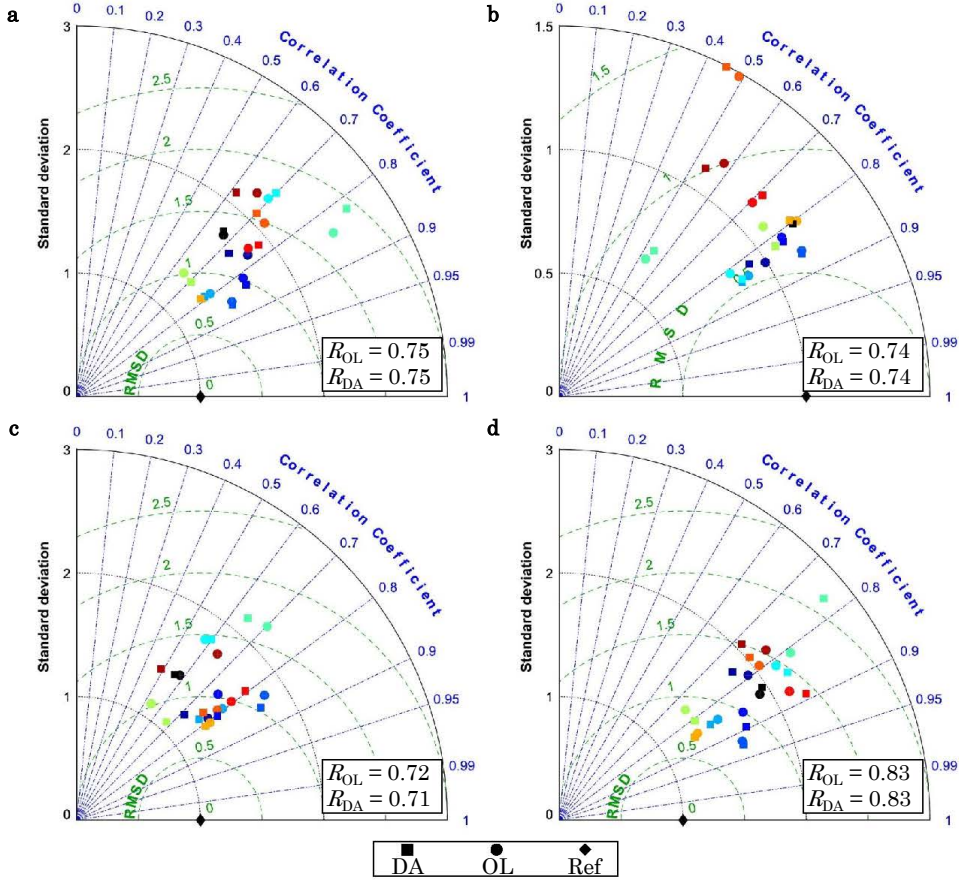


Figure 2.6: Taylor plots of the validation statistics of the modelled evaporation. Circles show the statistics for the open loop (OL) and corresponding statistics for the model run with assimilation (DA) of all SMOS data are shown as squares. The colours correspond to the different validation sites. Note that both the Root Mean Squared Difference (RMSD) and the standard deviation were normalised using the standard deviation of the observed time series such that the black diamond serves as a reference point for all other points. The average Pearson correlation coefficient (R) for all experiments is also reported. (a) Shows the validation of the 6-hourly simulations against the observed evaporation at the tower site, (b) shows the validation of the 6-hourly simulations against the energy residuals at the tower site, (c) shows the same statistics for the daily aggregates, and (d) shows the validation of the 6-hourly simulations when forcing the model with the tower-measured net radiation.

the energy residual at the towers as reference (note the different scale for the axis of the standard deviation). At the same time, also the RMSD is reduced. In addition, site differences in the correlation coefficients between Figures 2.6a

and b indicate that the differences between the direct observations of the latent heat flux and the energy residual are not simply systematic, which should raise awareness regarding the reliability of the in situ measurements. Nonetheless, large part of the mismatch between the model estimates and in situ reference will still relate to errors in model structure, parameterisation and forcing, as well as representativeness (point-to-pixel) errors.

From Figures 2.6a and b it becomes apparent that the impact of the assimilation algorithm on evaporation is neither large, nor it leads to systematic improvements across all towers. In general, the impact of assimilating SMOS retrievals on the modelled evaporation is low and can be either positive or negative. According to the results in Figure 2.6a, a statistical significant increase of the correlation coefficients at the 5% confidence level is observed at 5 out of 12 sites, while at an equal number of other stations correlation coefficients are significantly decreasing according to the statistical test. At two sites, no significant difference between both correlations could be shown. Nonetheless, these results are affected by the reduced availability of ground data, and the fact that towers are not always located in water-limited regimes (Figure 2.2) where the impact of the assimilation on evaporation is expected to be larger. Note that these results are consistent with Peters-Lidard *et al.* (2011), who assimilated AMSR-E data sets into different land surface models, and who could only observe a mild impact of the soil moisture assimilation on the modelled evaporation fields, especially during water-limited periods.

The results in Figure 2.6a correspond to the estimates at 6-hourly resolution. To test to what extent the observed correlations relate simply to the representation of the diurnal cycle, Figure 2.6c shows analogous results for the daily aggregates of evaporation. Due to the aggregation, the number of days with eddy-covariance measurements is reduced since only days with full data coverage are used to calculate the aggregates. As expected, the correlation coefficients mildly decrease, although the remaining statistics (RMSD and standard deviation) are improved. The impact of the assimilation algorithm on the daily estimates is comparable to the one on the 6-hourly simulations.

Finally, Figure 2.6d shows the results of forcing the model with tower-measured net radiation as opposed to radiation components derived from CERES as described in Section 2.3.1. Gaps in the in situ measurements of net radiation have been filled using a linear regression between the time series of CERES and the radiation measurements at the tower. Since precipitation is not measured at every site, an analogous substitution experiment cannot be done for precipitation. Unsurprisingly, the correlation coefficients generally increase to values of 0.83 on average, whereas the RMSD decreases, while the higher variability with respect to the direct in situ measurements of evaporation remains the same as in Figure 2.6a. Other experiments using a dynamic γ and assimilating only ascending or descending data were also conducted in this

study, but the same conclusions were obtained. Therefore, the results from these experiments are not shown.

Figure 2.7 shows time series of modelled terrestrial evaporation for the complete study period for sites AU-ASM (Figure 2.7a), AU-DaS (Figure 2.7b), and AU-Stp (Figure 2.7c), with the observed in situ data. For these figures, the combined ascending-descending SMOS data set was assimilated into GLEAM using a constant quality factor in the Newtonian Nudging scheme (Pearson correlation coefficients against the in situ data at all sites for this experiment are listed in Table A.1; Appendix A). For visual purposes only, all variables have been aggregated to daily intervals. The time series presented in Figure 2.7 confirm that the dynamics of the in situ measurements of evaporation are generally well captured by the model. Correlation coefficients between the OL simulation and the in situ measurements of 0.79, 0.83 and 0.81 are obtained for AU-ASM, AU-DaS, and AU-Stp, respectively. After assimilation of the complete SMOS data set, these correlation coefficients change to 0.71, 0.85 and 0.81 respectively. The lower correlation coefficient at AU-ASM potentially responds to errors in the descending SMOS data set at the site, since the assimilation of the ascending SMOS data only leads to a significant increase in the correlation coefficient to 0.81 instead. A similar difference in quality between both overpasses is observed for AU-Stp, as the assimilation of only the ascending data significantly increases the correlation to 0.82. In terms of RMSD, similar conclusions can be drawn: for site AU-ASM, the RMSD increases from $0.73 \text{ mm}\cdot\text{day}^{-1}$ to $0.75 \text{ mm}\cdot\text{day}^{-1}$ if the complete SMOS data set is assimilated, but if only the ascending data are assimilated, the RMSD decreases to $0.66 \text{ mm}\cdot\text{day}^{-1}$. For AU-DaS and AU-Stp the RMSD is reduced after the assimilation of the combined ascending-descending data; from $0.99 \text{ mm}\cdot\text{day}^{-1}$ to $0.90 \text{ mm}\cdot\text{day}^{-1}$ for AU-DaS, and from $0.87 \text{ mm}\cdot\text{day}^{-1}$ to $0.84 \text{ mm}\cdot\text{day}^{-1}$ for AU-Stp.

Although not directly clear from the overall statistics, the time series show that the impact of the assimilation of surface soil moisture (Figure 2.5) is directly propagated towards the modelled evaporation (Figure 2.7). An increase (decrease) of the modelled surface soil moisture results in an increase (decrease) of the evaporative flux. An improvement in the soil moisture, however, may not necessary yield a more realistic evaporation. It is also shown that the fluctuations in the modelled surface soil moisture that are introduced after the assimilation (Figure 2.5), are also present in the modelled time series of terrestrial evaporation (Figure 2.7). Finally, it should be emphasised that there are several periods where the assimilation has no impact on the modelled evaporation because there is no evaporative stress, as the simulated soil moisture exceeds the critical soil moisture (see grey shade in Figure 2.5 and Equation 2.2).

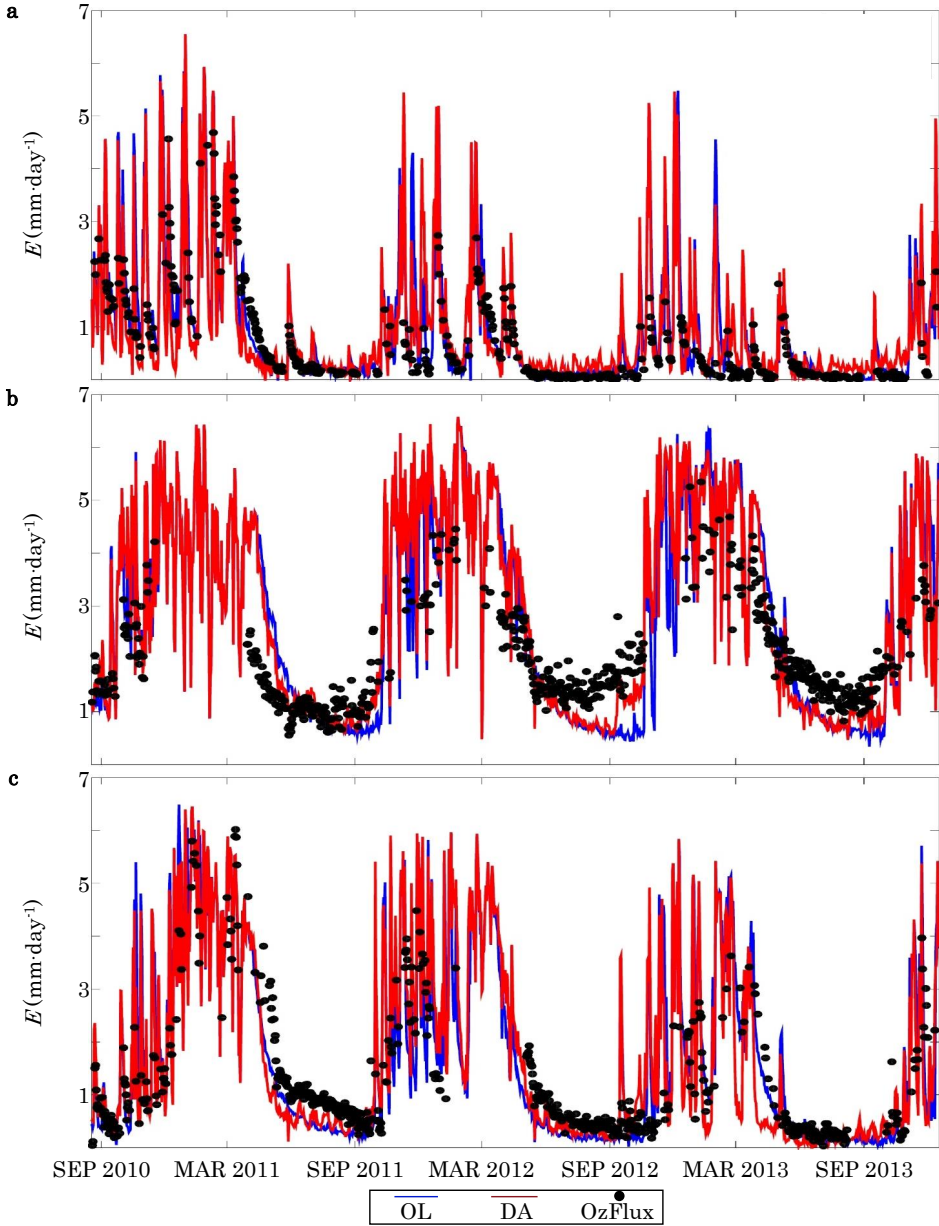


Figure 2.7: Time series of the modelled evaporation (E). For this experiment, the complete SMOS data set is assimilated into GLEAM and a constant quality factor is used in the assimilation algorithm. The simulations have been aggregated to daily scales for visual purposes. (a) Time series at site AU-ASM, (b) AU-DaS, and (c) AU-Stp.

2.5.4 Assimilation of AMSR-E soil moisture

For the overlap period September 2010 – October 2011, a comparison between the assimilation of SMOS and AMSR-E surface soil moisture into GLEAM can be conducted. For this sub-period, only 7 eddy-covariance sites report measurements of terrestrial evaporation, and 19 sites report soil moisture data. The results for the validation of the modelled surface soil moisture are presented in Figure 2.8. The red histograms show the results for SMOS, the results for AMSR-E are plotted in blue.

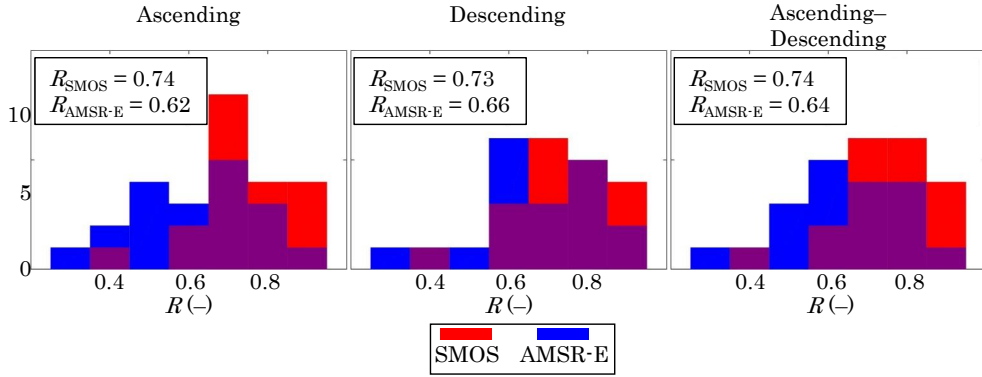


Figure 2.8: Histograms of the Pearson correlation coefficients (R) between the modelled and the in situ measured surface soil moisture at 19 validation sites. Histograms for the assimilation of AMSR-E are shown in blue and for the assimilation of SMOS in red. Where both histograms overlap, a purple colour is used. Separate histograms are shown for the assimilation of only ascending data, descending data, and both ascending and descending data. The average correlation coefficient for all experiments is also reported.

For this sub-period and subset of stations, the average Pearson correlation coefficient for the assimilation of the SMOS data is higher than when considering the entire multi-year study period (i.e. compared to Figure 2.4). The histograms for the correlations obtained with SMOS are consistently shifted towards the right in reference to the blue histogram of AMSR-E. This indicates that, on average, the quality of the SMOS soil moisture retrievals is higher, which is in agreement with the results of the TCA discussed in Section 2.5.1. Also the differences in data quality for different orbits is clear: for AMSR-E, the assimilation of descending data leads to significant improvements with respect to the assimilation of ascending data. These findings are in agreement with studies published by Su *et al.* (2013) and Draper *et al.* (2009), who also pointed out the lower accuracy of the ascending AMSR-E data. Nonetheless, the number of sites for which the assimilation of descending AMSR-E observations significantly improves the modelled surface soil moisture is only 4 out of 19,

while the assimilation of the combined ascending-descending product is not significantly improving the results at any of the sites. The explanation of this marginal positive impact of assimilating AMSR-E retrievals into GLEAM is twofold. First, the quality of the modelled surface soil moisture from the GLEAM OL is higher than that of the AMSR-E data: when the model simulations are restricted to time intervals with AMSR-E data (ascending or descending), the average correlation coefficient against in situ for the model OL is 0.64, while for AMSR-E the correlation against in situ measurements is only 0.49. For the descending data alone the correlation coefficient is higher (0.53) but still lower than the correlation of the model OL for the overlapping times (0.67). Second, in contrast to more complex algorithms, the Newtonian Nudging lacks the capability to correctly characterise and handle the (time-varying) uncertainties in both the modelled and observed state variables and their dependencies. While this was less restrictive for the assimilation of SMOS data, it is expected to have a higher impact for the assimilation of the AMSR-E data given the perceived lower quality of the data for Australia.

The effect of the assimilation of AMSR-E soil moisture on the modelled evaporation is summarised in Figure 2.9. Note that in these Taylor plots the circles represent the SMOS results, while the squares show the results for AMSR-E. As can be concluded from this figure, the validation results are similar from site to site, and usually indicate a higher performance by SMOS. Comparing Figures 2.9a and b shows that the statistics are slightly better for the assimilation of the descending AMSR-E data only. For sites AU-Dry (cyan color) and AU-GWW (black color), a larger difference can be observed; e.g. for AU-GWW the correlation remains unchanged, while the overestimation of the variability is strongly reduced after the AMSR-E data assimilation.

2.5.5 Continental-scale simulations

Maps of the modelled evaporation and soil moisture for continental Australia are presented in Figure 2.10. Figure 2.10a shows the results for the Austral winter of 2011 (June-July-August), while results for the Austral summer of 2010–2011 (December-January-February) are presented in Figure 2.10b. Top panels show the seasonal averages of terrestrial evaporation (E) and first ($w^{(1)}$), second ($w^{(2)}$), and third layer ($w^{(3)}$) soil moisture for the OL simulation. Remaining rows show the difference between the OL and the simulations with assimilation of SMOS or AMSR-E surface soil moisture, respectively. The spatial patterns of simulated fields are consistent with the climatological North-South transition from tropical climate to semiarid regime, and the magnitude of the modelled evaporative flux is realistic according to the results from independent studies (e.g. Jiménez *et al.*, 2011). Results for the Austral summer indicate an overall strong spatial correlation between the average modelled soil moisture and evaporation fields (with a spatial correlation

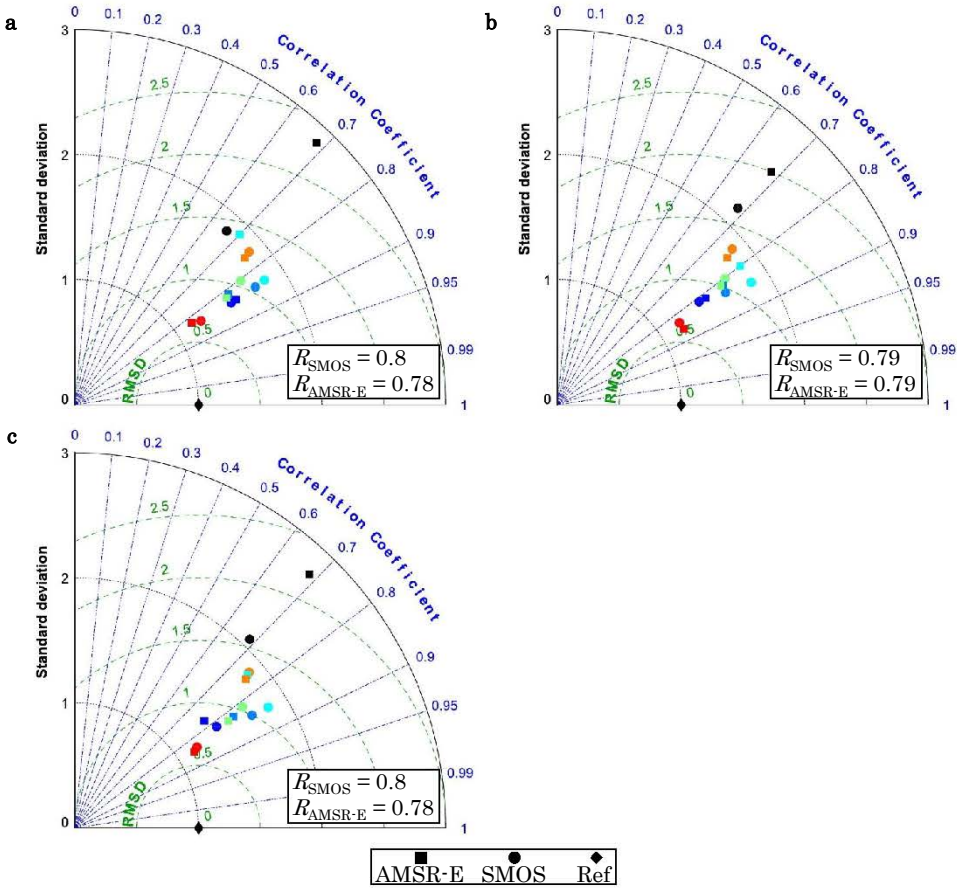


Figure 2.9: Taylor plots of the validation statistics of the modelled evaporation. Circles show the statistics for the assimilation of SMOS and corresponding statistics for the assimilation of AMSR-E are shown as squares. The colours correspond to the different validation sites. Note that both the Root Mean Squared Difference (RMSD) and the standard deviation were normalised using the standard deviation of the observed time series such that the black diamond serves as a reference point for all other points. The average correlation coefficient for all experiments is also reported. (a) Summarises the statistics after assimilating the ascending data only, (b) the same but for the descending data, and (c) the same but for the combined assimilation of ascending and descending data.

coefficient between the modelled evaporation in the OL and first-layer soil moisture of 0.60). For the Austral winter, this spatial agreement between the soil moisture and evaporation is lower (spatial correlation coefficient of 0.10). These results suggest that the ratio of the supply of vapour to the atmosphere and the atmospheric demand for water is larger in summertime, when potential

evaporation is also larger. While in the south the available energy is generally the limiting factor during the Austral winter, in the north the dry period also coincides with the period of lower radiation input (i.e. wintertime). This was already shown in the time series from Figures 2.5 and 2.7.

Although the impact on evaporation estimates of assimilating microwave soil moisture is not directly apparent from the statistics discussed in Section 2.5.3, the differences seen in Figure 2.10 demonstrate that this impact can in fact be quite substantial, with seasonal average differences in modelled fluxes reaching up to 100% for drier times and regions. This is especially the case for the assimilation of AMSR-E observations. This can only be explained by a seasonal mismatch in the soil moisture climatologies, which can still exist after the CDF-matching prior to the assimilation of the microwave soil moisture data (Section 2.2.2), and leads to larger innovations when assimilating AMSR-E data. This also explains the opposite impact of the assimilation of AMSR-E data during summer and winter months.

Finally, Figure 2.10 also shows that the calculated innovations at the first layer are propagated efficiently towards the other model layers, and that even in these deeper layers the impact of surface soil moisture assimilation can be equally high. A validation of the modelled soil moisture at deeper layers and the global application of the methodology will be the subject of Chapter 3.

2.6 Conclusion

The main objective of this chapter was to investigate the potential value of assimilating SMOS soil moisture to reduce the uncertainty in satellite-based model estimates of terrestrial evaporation and soil moisture from GLEAM. With this aim, GLEAM was used to simulate evaporation fields over continental Australia for the period September 2010 – December 2013. A simple Newtonian Nudging algorithm was implemented to assimilate the microwave soil moisture into the evaporation model. The modelled surface soil moisture and corresponding evaporation fields were validated against in situ measurements from 25 soil moisture probes and 12 eddy-covariance towers. The assimilation of SMOS data and the evaluation of the estimates of terrestrial evaporation and soil moisture offered an alternative way to evaluate the accuracy and value of SMOS observations for hydrological studies. Results obtained from the assimilation of SMOS soil moisture into GLEAM were compared to analogous results obtained through assimilation of AMSR-E retrievals for a one-year period.

Results point out that the soil moisture data retrieved from SMOS have the potential to improve the modelled soil moisture from GLEAM. If both the ascending and descending SMOS retrievals were assimilated, the modelled surface soil moisture could be significantly improved at 17 out of 25 individual

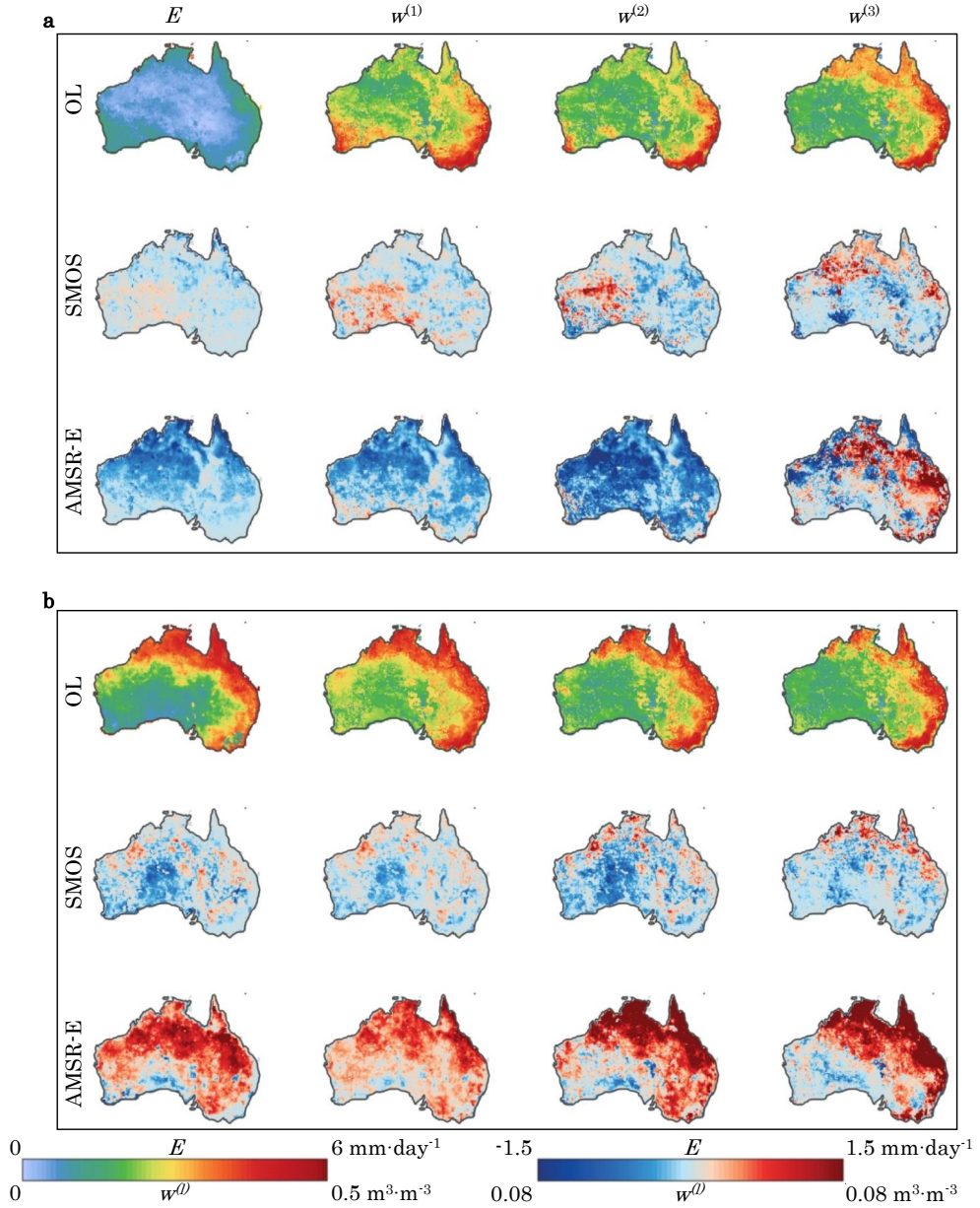


Figure 2.10: Continental maps of the average modelled evaporation (E) and soil moisture ($w^{(l)}$). Results are presented for the open loop (OL), AMSR-E data assimilation, and SMOS data assimilation separately. The latter two are shown in the form of differences with respect to the OL. **(a)** Maps for Austral summer (December-January-February) and **(b)** for Austral winter (June-July-August).

sites in terms of Pearson correlation coefficient. Contrary, the impact on the estimates of evaporation is difficult to evaluate. While the updates in soil moisture certainly propagate to the evaporation fields, the net effect on these estimates is not definitive. Moreover, the limited amount of in situ measurements of evaporation in water-limited regions (where soil moisture is expected to have the highest impact on terrestrial evaporation) prevents a more in depth evaluation of the value of SMOS data to improve evaporation estimates at this stage.

The quality of the SMOS observations was generally found to be higher than that of the AMSR-E data. This may in fact be explained by the sensing frequency of SMOS (L-band), specifically designed to retrieve surface soil moisture. While the C-band signal sensed by AMSR-E is relatively more contaminated by vegetation, hampering the retrieval of surface soil moisture. The difference in quality between the ascending and descending SMOS data appeared to be rather small, with the ascending being slightly better. Contrary, the assimilation of the ascending AMSR-E data, or the combined ascending-descending AMSR-E data set, generally decreased the model performance (for both soil moisture and evaporation). The lower quality of the ascending AMSR-E data relates to the strong temperature gradient at the time of data acquisition. The quality of the descending AMSR-E data has shown to be higher, allowing to improve the modelled soil moisture at only 4 out of 19 in situ stations. The inability of the AMSR-E data to significantly improve the modelled soil moisture was explained by the relatively lower quality of these data sets compared to the modelled soil moisture and the use of a simple assimilation algorithm.

The study also investigated the impact of the dynamics of observation and model errors on the performance of the assimilation scheme. It was concluded that the use of a dynamic quality factor in the Newtonian Nudging algorithm did not significantly improve the results compared to the use of a constant quality factor. These findings help to circumvent the need to run the model in ensemble mode to derive a dynamic model error, which has important implications in terms of computational demands when the model is applied globally and/or over multi-decadal periods. When a constant quality factor is used in GLEAM, only a TCA needs to be performed prior to the assimilation. However, these results are based on a limited set of validation sites and differences are minor. Moreover, the dynamic errors were retrieved using empirical, yet intuitive, methods which can be improved to objectively derive the temporal variability of both the model and observation errors.

CHAPTER 3

Estimating terrestrial evaporation at the global scale using GLEAM at coarse resolution

This chapter presents the third version of GLEAM (v3) and its changes relative to its predecessor. Key changes include: (1) a revised formulation of the evaporative stress, (2) an optimised drainage algorithm, and (3) a new soil moisture data assimilation system. GLEAM v3 is used to produce three new data sets of terrestrial evaporation and root-zone soil moisture, including a 36-year data set spanning 1980–2015, referred to as v3.0a (based on satellite-observed soil moisture, VOD, and snow-water equivalent, reanalysis air temperature and radiation, and a multi-source precipitation product), and two satellite-based data sets. The latter share most of their satellite-based forcing, except for the VOD and soil moisture, which are based on observations from different passive and active C- and L-band microwave sensors for the v3.0b data set (spanning 2003–2015), and observations from SMOS in the v3.0c data set (spanning 2011–2015). Here, these three data sets are described in detail, compared against analogous data sets generated using the previous version of GLEAM (v2), and validated against measurements from 91 eddy-covariance towers and 2325 soil moisture sensors across a broad range of ecosystems. This chapter is an edited version of the following scientific publication:

Martens, B., Miralles, D.G., Lievens, H., van der Schalie, R., de Jeu, R.A.M., Fernández-Prieto, D., Beck, H.E., Dorigo, W.A., Verhoest, N.E.C., 2017. GLEAM v3: satellite-based land evaporation and root-zone soil moisture. *Geoscientific Model Development* 10 (5), 1903–1925.

3.1 Introduction

Climate change alters the complex interplay between land and atmosphere, significantly impacting different processes in the global hydrological cycle (Miralles *et al.*, 2014; Wild *et al.*, 2008; Huntington, 2006). Analysing these impacts requires long-term, observational, and consistent data sets of essential hydrological variables, such as soil moisture, precipitation, and terrestrial evaporation. Unfortunately, the large-scale observation of terrestrial evaporation is hampered by the inability to sense this flux directly from satellites. The potential of satellite remote sensing to enhance our understanding of terrestrial evaporation dynamics has been intensively explored over the last decade (Section 1.1.4). While in the near future, evaporation will remain undetectable from space, several models that combine remotely-observable drivers of this flux (e.g. radiation, air temperature, soil moisture) have been developed and are being intensively used in recent years (Gomis-Cebolla *et al.*, 2019; Talsma *et al.*, 2018a; McCabe *et al.*, 2016; Michel *et al.*, 2016; Miralles *et al.*, 2016; Mueller *et al.*, 2013; Jiménez *et al.*, 2011).

GLEAM is arguably the only one of these global evaporation models that is designed to be driven by remote sensing observations alone; mainly obtained in the microwave domain. Evaporation and root-zone soil moisture data sets from GLEAM have been widely used in the past to study spatial variability and trends in the water cycle (e.g. Zhang *et al.*, 2016b; Greve *et al.*, 2014; Miralles *et al.*, 2014; Jasechko *et al.*, 2013), as well as land–atmosphere feedbacks (e.g. Guillod *et al.*, 2015; Miralles *et al.*, 2014). The first version (v1) of the model was developed by Miralles *et al.* (2011b) and further refined in 2014 (v2) by Miralles *et al.* (2014). Note that the latter version has been used and described in Chapter 2; this chapter presents the third version (v3) of the model. In this new version, most components of GLEAM have been updated, except for the interception loss algorithm and the potential evaporation module. First, aiming at a more realistic representation of evaporative stress, observations of microwave VOD and root-zone soil moisture have been combined to represent the non-linear response of soil and vegetation to the drying of land (e.g. Combe *et al.*, 2016; Ronda *et al.*, 2002; Serraj *et al.*, 1999; Colello *et al.*, 1998). Second, the soil module has been adapted to represent the continuous drainage of precipitation through the soil profile. Finally, the soil moisture data assimilation system, described in Section 2.2.2, has been optimised to work at the global scale and to integrate different data sets of satellite soil moisture observations. These changes have respected the minimalistic approach of GLEAM of targeting only the fundamental processes controlling large-scale evaporation rates, while keeping the overall simplicity and observational nature of the model.

The main goal of this chapter is to present the new version of GLEAM and the resulting evaporation and root-zone soil moisture data sets, including a

global validation using a large data base of soil moisture measurements from 2325 in situ sensors, and evaporation measurements from 91 eddy-covariance towers. In addition, the quality of these data sets is compared against analogous data sets generated using the former version of GLEAM, allowing to evaluate the added value of the new model formulations. The chapter is organised as follows: Section 3.2 describes the new algorithms, highlighting the main changes upon the previous version. The forcing data and the in situ validation data are described in Section 3.3. Section 3.5 analyses the quality of the GLEAM data sets and discusses the results, while the main conclusions are summarised in Section 3.6.

3.2 Advances in GLEAM

The baseline description of GLEAM is provided in Section 2.2.1, a detailed description of GLEAM v1 is given in Miralles *et al.* (2011b) and Miralles *et al.* (2010), and GLEAM v2 is described in Miralles *et al.* (2014). In this section, the changes relative to GLEAM v2 (Section 2.2.1) are described, and this new version is referred to as GLEAM v3. Note that an overview of the forcing variables in the model is given in Table 3.1.

3.2.1 Soil module

Figure 3.1 shows a schematic of the conceptual root zone for the fraction of tall vegetation in a grid cell of GLEAM. Note that, as described in Section 2.2.1, the root zone for the fraction of short vegetation only contains two soil layers, and that the fraction of bare soil is represented by only one soil layer. Each soil layer is conceptually subdivided into three different compartments. The first compartment (bottom) represents the water retained below the wilting point which is not available for root uptake; for the bare soil fraction, the residual soil moisture, w_r ($\text{m}^3 \cdot \text{m}^{-3}$), is used instead. The second compartment of the layer is bounded by the wilting point and the porosity ($\text{m}^3 \cdot \text{m}^{-3}$) of the soil matrix, w_p , and represents the maximum volume of water available for evaporation. Finally, the third compartment represents the solid phase of the soil column and thus cannot hold any water. At every time step t , the state of any layer l is characterised by its water content $w_t^{(l)}$ ($\text{m}^3 \cdot \text{m}^{-3}$), which is updated using:

$$w_t^{(l)} = w_{t-1}^{(l)} + \frac{\left(F_{s,t}^{(l-1)} + F_{f,t}^{(l-1)} - E_{t-1}^{(l)} - F_{s,t}^{(l)}\right) \Delta t}{\Delta z^{(l)}}, \quad (3.1)$$

where $w_{t-1}^{(l)}$ is the volumetric soil moisture content ($\text{m}^3 \cdot \text{m}^{-3}$) of layer l at the previous time step ($t-1$), $F_{s,t}^{(l-1)}$ is the volume of water per unit area slowly draining into the layer (slow draining flux, $\text{m} \cdot \text{s}^{-1}$), $F_{f,t}^{(l-1)}$ is the volume of

water per unit area directly reaching the layer (fast draining flux, $\text{m}\cdot\text{s}^{-1}$), $E_{t-1}^{(l)}$ is the evaporative flux from the previous time step to be extracted from the soil layer ($\text{m}\cdot\text{s}^{-1}$), $F_{s,t}^{(l)}$ is the slow drainage of water out of the soil layer ($\text{m}\cdot\text{s}^{-1}$), Δt is the length of a model time step (s), and $\Delta z^{(l)}$ is the depth of the soil layer (m) under consideration. Note that for the first layer ($l=1$), only $F_{f,t}^0$ is considered as an input, as there is no draining layer on top.

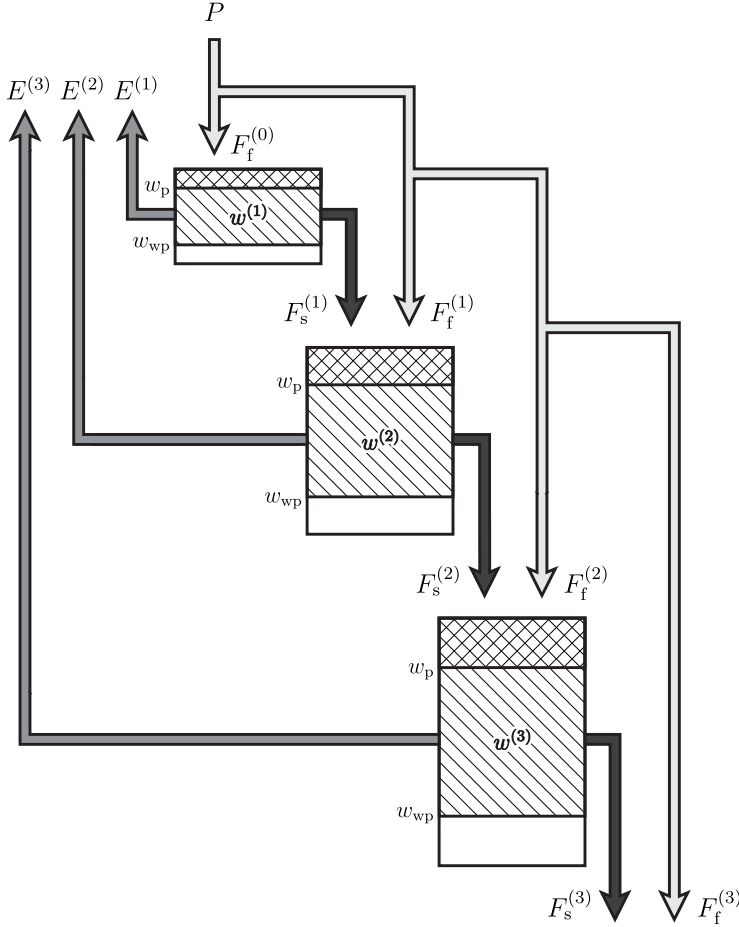


Figure 3.1: Schematic representation of the soil module implemented in GLEAM v3 for the fraction of tall vegetation. $w^{(l)}$ is the volumetric soil moisture content ($\text{m}^3\cdot\text{m}^{-3}$) of layer l , $F_s^{(l)}$ is the slow draining volume of water ($\text{m}\cdot\text{s}^{-1}$), $F_f^{(l)}$ is the fast draining volume of water ($\text{m}\cdot\text{s}^{-1}$), $E^{(l)}$ is the evaporative flux ($\text{m}\cdot\text{s}^{-1}$), P is the net precipitation ($\text{m}\cdot\text{s}^{-1}$), w_{wp} is the wilting point ($\text{m}^3\cdot\text{m}^{-3}$) and w_p is the porosity ($\text{m}^3\cdot\text{m}^{-3}$).

In previous model versions, the entire volume of net precipitation (i.e. precipitation minus interception loss, plus snowmelt) was first stored in the top layer, which subsequently drained to field capacity into the next soil layer

(Section 2.2.1); the same process was used to calculate the vertical flow from the remaining layers. As a result, the soil moisture could not exceed field capacity, nor was drainage allowed to occur below that threshold. In GLEAM v3, net precipitation is first partitioned between the different soil layers based on the relative saturation at the beginning of the time step, in order to estimate the fast draining flux $F_{f,t}^{(l)}$. Next, the volume of water that slowly drains to the next layer ($F_{s,t}^{(l)}$) is estimated using a simplified representation of Darcy’s law, in which a fraction of the available water above wilting point is drained to the next layer based on (1) the relative saturation of each layer, and (2) the difference in soil moisture content between both layers. The rationale behind this simple drainage algorithm is that the downward flux of water is expected to increase if (1) the relative soil moisture content is higher (physically resulting in increased hydraulic conductivities), and (2) the difference in soil moisture between source and sink is larger (resulting in higher differences in soil-water potential). This empirical drainage algorithm is preferred over well-known alternatives such as the Richards equation (Richards, 1931), Brooks-Corey (Brooks and Corey, 1964), or Clapp-Hornberger (Clapp and Hornberger, 1978), due to its simplicity and the fact that it does not require the use of additional, largely-unconstrained, ancillary data on soil properties at the global scale.

3.2.2 Data assimilation system

The original Kalman filter approach to assimilate microwave soil moisture observations – typically sensitive to the first few centimeters of the soil (Schmugge, 1983) – into GLEAM was replaced in favour of a simple Newtonian Nudging algorithm in the v2 (Miralles *et al.*, 2014), which was further optimised in Chapter 2. This Newtonian Nudging scheme minimises the computational demands and fits well within the rationale of GLEAM of keeping the model as simple and observation-driven as possible. While more complex algorithms like the ensemble Kalman filter have also been applied in GLEAM, the added value has shown to be marginal (Miralles *et al.*, 2014). Therefore, in this new version, a similar approach to the Newtonian Nudging scheme described in Section 2.2.2 is adopted:

$$\hat{w}^{(1)+} = \hat{w}^{(1)-} + K\gamma \left(\langle w^o \rangle - \langle \hat{w}^{(1)-} \rangle \right), \quad (3.2)$$

where $\langle w^o \rangle$ and $\langle \hat{w}^{(1)-} \rangle$ are the observed and modelled soil moisture anomalies, respectively. The latter represent deviations relative to the seasonal climatology of soil moisture – calculated as in Lievens *et al.* (2017) and De Lannoy and Reichle (2016) – as opposed to the absolute values of soil moisture assimilated in Chapter 2. K is still set to a value of 1 to maximise the impact of the assimilation algorithm as in Chapter 2. Note that as compared to

Equation 2.5, the interpolation weight $W^{(l)}$ is also dropped here, as the innovation ($\langle w^o \rangle - \langle \hat{w}^{(1)-} \rangle$) directly corresponds to the state of interest (i.e. the soil moisture of the first layer), and $W^{(1)}$ thus equals one.

As most assimilation algorithms require bias-free observations in reference to the modelled states, a bias removal algorithm prior to (or during) the assimilation step has to be applied (Section 2.2.2). However, no standard procedure exists to correct these constant or seasonally varying biases (De Lannoy and Reichle, 2016; Lievens *et al.*, 2015), thus the choice of the bias-removal algorithm remains to some degree subjective. As indicated in Section 2.5.5, the use of a classical CDF-matching approach prior to the assimilation step introduced seasonal biases in the GLEAM soil moisture and evaporative fluxes. As a result, in GLEAM v3, soil moisture anomalies are assimilated instead, as this approach allows the correction of potential seasonal biases between the modelled and observed soil moisture states (De Lannoy and Reichle, 2016). As a TCA (Gruber *et al.*, 2016; Miralles *et al.*, 2010; Scipal *et al.*, 2008) is applied here to obtain the observation and model errors, the anomaly time series of the observations are scaled towards the modelled soil moisture anomalies using a linear regression model prior to the assimilation (Yilmaz and Crow, 2013). The three independent and rescaled anomaly time series of surface soil moisture are then applied in the TCA to estimate both the random model and observation errors. In contrast to the TCA described in Section 2.2.2, TCA is applied here on a yearly basis to capture temporal changes in microwave soil moisture accuracy due to scientific and technological advances. The two errors are then adopted to calculate the quality factor (γ) using Equation 2.6.

Finally, in contrast to the assimilation of soil moisture observations in all model layers in Chapter 2, only the first model layer is updated here, as shown in Equation 3.2. The latter choice is motivated by the slower dynamics of the deeper model layers, which are strongly perturbed when soil moisture observations are directly assimilated into these layers using the simple Newtonian Nudging scheme. The impact of the soil moisture update in GLEAM v3 is thus propagated towards deeper layers by drainage processes only, which ensures a smooth transition of water through the vertical profile.

3.2.3 Stress module

Water availability, heat stress, or phenological constraints affecting the rate at which water can be supplied from the land surface to the atmosphere, are generally combined in a single empirical stress factor accounting for the decrease in potential evaporation (Combe *et al.*, 2016; Sellers *et al.*, 2007). In GLEAM, a multiplicative stress factor S ranging between 0 (maximum stress and thus no evaporation) and 1 (no stress and thus potential evaporation) is defined (Section 2.2.1). In the first version (Miralles *et al.*, 2011b), S was parameterised separately for the fractions of tall and short vegetation using

non-linear relationships between S and the soil moisture of the wettest layer. To account for changes in vegetation phenology of short vegetation, the VOD was also used in the calculation of S for this fraction. These functions were linearised in the second version, and the VOD was also introduced for the calculation of the stress for the fraction of tall vegetation (Miralles *et al.*, 2014). However, based on experimental evidence, a non-linear response of S to soil moisture is expected for most vegetation types (e.g. Combe *et al.*, 2016; Ronda *et al.*, 2002; Serraj *et al.*, 1999; Colello *et al.*, 1998). Hence, a non-linear stress function for both tall and short vegetation is re-introduced in GLEAM v3:

$$S = \sqrt{\frac{\vartheta}{\vartheta_{\max}}} \left(1 - \left(\frac{w_c - w^{(w)}}{w_c - w_{wp}} \right)^2 \right) \quad (3.3)$$

As soil moisture decreases, S decreases (i.e. increased evaporative stress), since water becomes less easily available for the roots. As vegetation phenology is not explicitly accounted for, the VOD – closely linked to the vegetation water content (Liu *et al.*, 2013) – is used to account for the effect of (seasonal or occasional) phenological constraints on evaporation (e.g. leaf-out, fires, pests), with decreasing VOD resulting in lower values for S and thus higher evaporative stress. As seen from Equation 3.3 and Figure 3.2, the stress function is thus affected by both the soil moisture content in the wettest soil layer and the VOD. If $w^{(w)}$ reaches w_{wp} , Equation 3.3 implies that the vegetation is incapable of retrieving water from the soil and S equals zero (and so does actual transpiration, Equation 2.3). Contrary, for soil moisture values exceeding w_c and the VOD reaching its maximum value, it is assumed that the vegetation is unstressed (i.e. $S = 1$, thus transpiration equals potential transpiration, Equation 2.3).

Figure 3.2 illustrates the shape of the stress function described by Equation 3.3 for a grid cell dominated by a strong seasonality in VOD (Figure 3.2a) and a site with a limited variability in VOD (Figure 3.2b). For illustrative purposes only, it is assumed that the soil properties (w_c and w_{wp}) are the same for both sites. As can be seen, where the range in VOD is low given the absence of a marked seasonality, S mainly depends on soil moisture. Conversely, if a large seasonality in the VOD is present (Figure 3.2a), the VOD becomes more important for the calculation of S .

Finally, for the bare soil fraction, S is linearly related to the soil moisture state using the critical and residual soil moisture content as upper and lower boundary conditions, respectively:

$$S = 1 - \frac{w_c - w^{(1)}}{w_c - w_r} \quad (3.4)$$

Since only the top layer is considered for the fraction of bare soil, S is fully driven by surface soil moisture ($w^{(1)}$) alone.

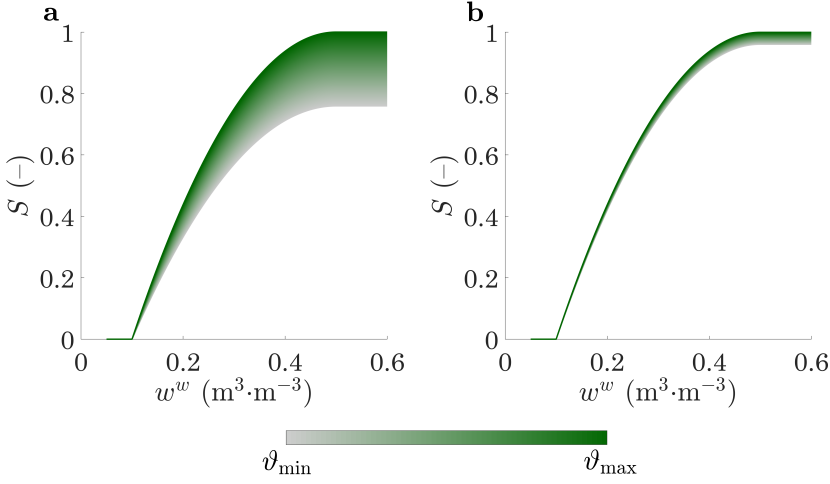


Figure 3.2: Illustration of the stress function implemented in GLEAM v3 for the vegetated fractions. For illustrative purposes only, the wilting point and the critical soil moisture for both figures were set to 0.1 and 0.5 $\text{m}^3 \cdot \text{m}^{-3}$, respectively. **(a)** For a grid cell with a high range in VOD ($\vartheta_{\max} = 0.47$, $\vartheta_{\min} = 0.27$), and **(b)** for a grid cell with a small range in VOD ($\vartheta_{\max} = 0.40$, $\vartheta_{\min} = 0.38$).

3.3 Data

3.3.1 Input data sets

Table 3.1 gives an overview of the selected forcing data sets in GLEAM v3. All input data sets have a daily resolution and are linearly resampled from their original spatial resolution to a common 0.25° global grid. Given the aim to extract all valuable information on terrestrial evaporation from existing satellite records, forcing data sets are preferentially derived from satellite observations. However, since a key application of the GLEAM data sets is to analyse the impact of climate change on terrestrial hydrology, the use of alternative forcing data sets, such as reanalysis data, to yield multi-decadal records of terrestrial evaporation and root-zone soil moisture is also explored here.

Table 3.1: List of the selected forcing data sets together with an indication of the type of data, their approximate native spatial and temporal resolution, and their reference. The first column indicates the use of these data in GLEAM.

GLEAM data set	Variable	Data set	Type	Resolution		References
				Spatial	Temporal	
v3.0b,c	Radiation	CERES L3 SYN1DEG Ed4A	Satellite	110 km	3 hours	Doeling (2017)
v3.0a		ERA-I	Reanalysis	80 km	6 hours	Dee <i>et al.</i> (2011)
v3.0b,c	Precipitation	TRMM 3B42 v7	Merge	27 km	3 hours	NASA GES DISC (2018)
v3.0a		MSWEP v1.0	Merge	27 km	1 day	Beck <i>et al.</i> (2017)
v3.0b,c	Temperature	AIRS L3RetStdv6.0	Satellite	110 km	1 day	Texeira (2013)
v3.0a		ERA-Interim	Reanalysis	80 km	3 hours	Dee <i>et al.</i> (2011)
v3.0a-c	Snow	GLOBESNOW L3av2	Satellite	27 km	1 day	Luojus <i>et al.</i> (2013)
		NSIDC v0.1			1 month	Armstrong <i>et al.</i> (2005)
v3.0c	VOD	SMOS-LPRM	Satellite	27 km	3 days	van der Schalie <i>et al.</i> (2015b,a)
v3.0a,b		CCI-LPRM	Satellite	80 km	1 day	Liu <i>et al.</i> (2011, 2013)
v3.0c	Soil moisture	SMOS L3	Satellite	25 km	3 day	Jacquette <i>et al.</i> (2010)
v3.0a,b		ESA CCI SM v2.3	Satellite	25 km	1 day	Liu <i>et al.</i> (2012); Wagner <i>et al.</i> (2012)
v3.0a-c		GLDAS Noah	Reanalysis	110 km	3 hours	Rodell (2007)
v3.0a-c	Cover fractions	MOD44B v51	Satellite	250 m	1 year	Dimiceli <i>et al.</i> (2015b)
v3.0a-c	Soil properties	IGBP-DIS	Survey	27 km	static	Global Soil Data Task Group (2000)
v3.0a-c	Lightning	LIS/OTD	Satellite	5 km	1 month	Cecil <i>et al.</i> (2014)

Radiation inputs are based on measurements from CERES onboard Terra and Aqua (Wielicki, 1996), which are available globally from the year 2001 onwards on a 1° regular grid in the CERES L3 SYN1DEG Ed4A product (Doelling, 2017). Additionally, radiation fluxes from ECMWF’s ERA-I data set (Dee *et al.*, 2011) are also processed. ERA-I data are available globally from 1979 to present, with a temporal resolution of 3 hours and a spatial resolution of approximately 0.75° . For the precipitation forcing, the TRMM 3B42v7 product (NASA GES DISC, 2018) produced by Huffman *et al.* (2007) and the Multi-Source Weighted-Ensemble Precipitation (MSWEP) data set (Beck *et al.*, 2017) are selected. The former data set combines measurements from several satellites and is bias corrected on a monthly time scale using ground-based measurements of precipitation. The product is available for the period 1998–2015 and covers 50°N – 50°S based on a 0.25° grid. MSWEP is a merger of selected satellite-, reanalysis- and gauge-based products, and is available from 1979 until 2015 at a 0.25° spatial resolution. Air temperatures are derived from measurements of the Atmospheric Infrared Sounder (AIRS; Aumann *et al.*, 2003), which are available from 2003 onwards on a global 1° regular grid in the AIRS L3RetStdv6.0 product (Texeira, 2013). Air temperature estimates from ERA-I are also selected for the long-term GLEAM data set. As for the radiation, data are available globally from 1979 until near present at 3-hourly intervals. To estimate sublimation, observations of snow-water equivalent from the ESA GLOBSNOW product (Luo *et al.*, 2013) are used. This data set is mainly based on retrievals from the Scanning Multichannel Microwave Radiometer (SMMR), Special Sensor Microwave/Imager (SSM/I), and AMSR-E, and in situ snow measurements. The data set is available from 1980 onwards and only covers the Northern Hemisphere. Therefore, the GLOBSNOW product is merged here with the National Snow and Ice Data Center (NSIDC) monthly snow-water equivalent climatology product (Armstrong *et al.*, 2005) for the Southern Hemisphere. The latter is also based on measurements from SMMR and SSM/I.

As discussed in Section 3.2.3, the phenological controls on transpiration are derived from observations of microwave VOD. Here, the 0.25° product from Liu *et al.* (2011) is used, which is based on retrievals from several passive microwave sensors using LPRM (Owe *et al.*, 2008). The product is available at the global scale and spans the period 1980–2012; in order to cover the period 1980–2015, it is merged with LPRM-based VOD retrievals from SMOS (van der Schalie *et al.*, 2015b,a) using a similar CDF-matching approach as the one used by Liu *et al.* (2011). The resulting data set contains gaps due to the repeating cycle of the satellites, the requirement of non-frozen conditions for parameter retrieval, and the presence of radio frequency interference. In order to obtain smooth and continuous time series, the VOD data set is gap-filled using a moving average filter with a 7-day window. Remaining gaps, generally occurring in winter time

due to freezing temperatures and snow covers, are linearly interpolated between the last and next available retrieval. Note however that in periods for which the land is covered by snow, the VOD is not used as the entire evaporation flux is assumed to be sublimation in that case (Section 2.2.1). Finally, if any gaps remain, these are filled using nearest neighbour interpolation. It should be noted here that microwave sensors operating at different frequencies might be sensitive to diverse components of vegetation, varying at different time scales (e.g. Liu *et al.*, 2011; Guglielmetti *et al.*, 2007). Despite the CDF-matching, which corrects for differences in long-term statistics, the use of different microwave sensors might impact the temporal dynamics of the VOD data set used here.

Finally, for the assimilation of microwave surface soil moisture, the SMOS Level 3 soil moisture product (Jacquette *et al.*, 2010), and the ESA Climate Change Initiative soil moisture (ESA CCI SM v2.3) data set (Liu *et al.*, 2012; Wagner *et al.*, 2012) are selected. The latter is a blended product of soil moisture retrievals from several active and passive microwave sensors, available for the period 1978–2015 at the global scale. In addition, surface soil moisture fields from the Noah model in the Global Land Data Assimilation System (GLDAS; Rodell *et al.*, 2004) are used as a third independent data set in the TCA. Despite fundamental differences between GLEAM and Noah, some degree of dependency between their soil moisture estimates might be present due to the presence of common precipitation observations embedded within MSWEP, TRMM 3B42, and the forcing of GLDAS Noah. However, the merging schemes used to produce the precipitation data sets are ultimately different (Beck *et al.*, 2017; Huffman *et al.*, 2007; Rodell *et al.*, 2004). Such a dependency could penalise the satellite-based soil moisture in the TCA (Yilmaz and Crow, 2014), which would result in a lower quality factor γ (Equation 2.6) applied in the data assimilation system and, subsequently, in a more conservative soil moisture update. Note that there is also a dependency between GLDAS-Noah and ESA CCI as the former is used to derive the reference climatology in the merging scheme of the latter product (Gruber *et al.*, 2019). However, this is not expected to affect the TCA as GLDAS-Noah is only used in the merging as a bias-correction, while TCA estimates the random error in each data set (Section 3.2.2).

As discussed in Section 2.2.1, GLEAM also requires several static data sets describing the soil properties, average rainfall climatology, and land cover. For the former two, the same data sets as in Section 2.3.1 are used here, while for the land cover fractions the MODIS Global Vegetation Continuous Fields product (MOD44B) is selected (Hansen *et al.*, 2005) at 250 m instead of the coarse-scale 0.25° product described in Section 2.3.1. The high-resolution product is upscaled to the required grid size of 0.25° by simple averaging. Note that also in previous model versions, the low resolution 0.25° product

produced by the MODIS team was used instead. For the fraction of open water, the product produced by Tuanmu and Jetz (2014) is combined with the MODIS-based product.

Using various combinations of the forcing data, three different data sets of terrestrial evaporation and root-zone soil moisture are produced using GLEAM v3 (Table 3.1). The inputs of snow-water equivalent, the third independent data set used in the TCA, and the static fields are shared by all data sets. The first GLEAM data set (hereafter referred to as v3.0a) is a 36-year data set (1980–2015) covering the entire globe and is based on satellite-observed soil moisture, VOD, and snow-water equivalent, reanalysis air temperature and radiation, and the MSWEP data set for precipitation. Given the multi-decadal coverage of this data set, it is intended to foster climatological research. The remaining data sets (v3.0b and v3.0c) are driven by satellite-based data only, and span a shorter period. In addition, these data sets only cover 50°N–50°S due to the use of the TRMM 3B42v7 product. The differences between both satellite-based data sets are the VOD and soil moisture forcing, which are retrieved from multiple active and passive microwave sensors in the v3.0b data set, and from SMOS only in the v3.0c data set. This also implies a different record length of 13 (2003–2015) and 5 years (2011–2015) for the v3.0b and v3.0c data sets, respectively.

3.3.2 Validation data sets

For validation purposes, in situ soil moisture and evaporation measurements from different global networks are processed. As in Section 2.3.2, soil moisture measurements are sourced from the data base of the ISMN (Dorigo *et al.*, 2013, 2011), but all in situ sites are considered for inclusion in the validation data set in this chapter. In situ measurements of terrestrial evaporation are obtained from the FLUXNET 2015 synthesis data set (<http://fluxnet.fluxdata.org/>; last visit: 28 October 2019). An overview of the selected sites can be found in Table A.2 (Appendix A). All available measurements for 1980–2015 are considered for inclusion in the validation set. In situ measurements are largely processed as in Section 2.3.2, but soil moisture measurements are additionally masked for snow and air temperatures below 0°C using the snow-water equivalent from GLOBSNOW and the air temperature data sets, respectively (Table 3.1). Furthermore, time series are aggregated here to a daily temporal resolution, allowing 20% of the higher resolution data within the aggregation interval to be missing. Finally, only sites with at least 365 daily measurements after masking are included in the validation data set. This yields a total of 91 quality-checked eddy-covariance sites covering roughly 740 site years (Table A.2, Appendix A) and a total of 2325 soil moisture sensors covering various ecosystems across the globe. Note that the soil moisture sensors are installed at different depths below the soil surface and used to validate

both the first (0–10 cm, 1119 sensors) and second (10–100 cm, 1216 sensors) model layer, depending on the installation depth. As opposed to Section 2.3.2, sensors located in the same GLEAM grid cell (horizontally or vertically) are not combined here, but treated separately in the validation to avoid problems with potential artifacts resulting from merging sensors with different absolute values and gaps in their record. The location of the in situ sites selected in this study is shown in Figures 3.3 and 3.6 for the soil moisture sensors and eddy-covariance sites, respectively.

3.4 Experimental setup

In this chapter, GLEAM is run at the global scale at a spatial resolution of 0.25° and daily temporal time steps. Using various combinations of input data, three different data sets of terrestrial evaporation and root-zone soil moisture are produced as described in Section 3.3.1. For the long-term simulation (v3.0a), the model is initialised using the climatology of the first model time step calculated on a 15-year GLEAM run where the soil moisture of each model layer in GLEAM was initialised as the average of the wilting point and field capacity in the grid cell (similar to the approach described in Section 2.4). The two satellite-based data sets are initialised using the corresponding simulation in the v3.0a data set; i.e. the soil moisture from the v3.0a data set at the first day of the year in 2003 and 2011 for v3.0b and v3.0c, respectively. As in Section 2.4, the effect of the model initialisation is removed by taking into account a spin-up period in the validation. However, given the longer study period in this chapter, a spin-up period of one year is taken into account.

The estimated soil moisture in the first and second model layer of GLEAM, as well as the estimated terrestrial evaporation at daily time steps are evaluated against in situ measurements (Section 3.3.2) using the Pearson correlation coefficient and the unbiased RMSD (ubRMSD) as validation metrics. The quality of the three data sets is compared against each other, as well as against a simulation with GLEAM v2 using the same input data sets. To assess the impact of the optimised data assimilation system implemented in GLEAM (Section 3.2.2), validation statistics of the OL and the run with data assimilation are compared. Finally, a time series analysis at two selected focus sites is performed, the spatial patterns at the global scale are analysed, and the total volume of terrestrial evaporation and its partitioning into its components are compared between GLEAM v2 and GLEAM v3.

3.5 Results and discussion

3.5.1 Validation of soil moisture

Accuracy of soil moisture estimates

Table 3.2 summarises the average Pearson correlation coefficient and ubRMSD for the v3 soil moisture data sets against the in situ measurements. Validation statistics are calculated using all available in situ measurements within the spatio-temporal domain of each of the data sets, as well as using a common set of soil moisture sites and an overlapping period for the three data sets (i.e. 2011–2015). Statistics for analogous data sets obtained using GLEAM v2 (same input data, except for the MODIS land cover fractions) are shown between brackets for comparison. Differences in correlations for the three products are statistically tested for significance using a Student’s t-test (at the 10% level), after applying a Fisher Z transformation on the time series. The autocorrelation of the daily time series was taken into account by reducing the degrees of freedom of the test statistic using an effective sampling size as in Lievens *et al.* (2017) and De Lannoy and Reichle (2016)¹. Note that the first year of each of the data sets is not taken into account for this validation exercise to avoid the effects of model initialisation on validation statistics.

Table 3.2: Average validation statistics for the different soil moisture data sets (v3.0a–c) and for the first two model layers ($w^{(1)}$ and $w^{(2)}$) against in situ measurements: ubRMSD is the unbiased Root Mean Squared Difference, R is the Pearson correlation coefficient, and N is the number of sites included in the sample. The first part of the table reports the averaged statistics over all available sites and the entire study period, while the second part shows the same statistics for a common sample of sites, and an overlapping study period (2011–2015) for the three data sets. The same statistics for the data sets produced using GLEAM v2 are reported between brackets.

		Complete record			Overlap period		
		N	ubRMSD	R	N	ubRMSD	R
		(–)	($\text{m}^3 \cdot \text{m}^{-3}$)	(–)	(–)	($\text{m}^3 \cdot \text{m}^{-3}$)	(–)
v3.0a	$w^{(1)}$	1119	0.059 (0.060)	0.64 (0.61)	777	0.057 (0.062)	0.67 (0.62)
	$w^{(2)}$	1216	0.048 (0.051)	0.53 (0.47)	746	0.048 (0.054)	0.51 (0.44)
v3.0b	$w^{(1)}$	1038	0.061 (0.063)	0.61 (0.58)	777	0.060 (0.063)	0.62 (0.58)
	$w^{(2)}$	1129	0.049 (0.052)	0.49 (0.42)	746	0.049 (0.054)	0.49 (0.42)
v3.0c	$w^{(1)}$	785	0.059 (0.063)	0.63 (0.58)	777	0.060 (0.062)	0.63 (0.59)
	$w^{(2)}$	754	0.048 (0.052)	0.49 (0.42)	746	0.049 (0.052)	0.49 (0.44)

¹Note that the statistical test introduced here is different from the one used in Chapter 2, but is essentially assessing the same hypotheses. This is due to scientific advances made after the publication of Martens *et al.* (2016), from which e.g. Lievens *et al.* (2017) and De Lannoy and Reichle (2016) concluded that the statistical test used in this chapter should produce a more robust analysis.

As indicated by the statistics in Table 3.2, all data sets compare reasonably well against the in situ measured soil moisture, with correlations for the first model layer ($w^{(1)}$) of 0.64, 0.61 and 0.63 for the v3.0a, v3.0b, and v3.0c data sets, respectively. For the second model layer ($w^{(2)}$), correlations are lower (ranging from 0.49 to 0.53), which can be expected given the lower representativeness of a single in situ measurement over the thicker model layer (10–100 cm). The ubRMSD yields mean values of approximately $0.06 \text{ m}^3 \cdot \text{m}^{-3}$ and $0.05 \text{ m}^3 \cdot \text{m}^{-3}$ for the first and second model layer, respectively. Overall, the validation statistics shown in Table 3.2 point to a higher quality of the v3.0a soil moisture than that of the v3.0b and v3.0c. This is also confirmed by the statistics obtained for the common validation period: for both model layers and in terms of correlations, the v3.0a soil moisture is superior, with correlation coefficients for $w^{(1)}$ being significantly higher in approximately 20% of the sites (the opposite is true in 2% of the sites only). Due to the high autocorrelation in the second layer soil moisture – strongly reducing the degrees of freedom in the statistical test – correlations for the v3.0a data set are only higher at approximately 3% of the individual sites. Permutations of the precipitation forcing amongst the different data sets indicate that the higher quality of the soil moisture in v3.0a is primarily due to the precipitation forcing used in each data set (not shown), and suggests an overall high accuracy of the MSWEP data as indicated by Beck *et al.* (2017). Note, however, that more than 75% of the soil moisture probes are located in the Continental United States (CONUS), where gauge-based precipitation data sets are known to over-perform satellite-based products (Beck *et al.*, 2017). These findings should thus not be extrapolated to other regions. Finally, the difference in quality between v3.0b and v3.0c is relatively small, with slightly better statistics for the v3.0c data set, which integrates SMOS data.

For comparison, Table 3.2 also reports the validation statistics for the same data sets obtained using GLEAM v2. Both the ubRMSD and the correlation suggest that the v3 soil moisture data sets have a higher quality: at 26%, 19%, and 12% of the in situ soil moisture sites, the correlations significantly improve in case of the v3.0a, v3.0b and v3.0c data sets, respectively (statistically significant deterioration only occurs in a small number of sites). Although for the second layer significant improvements of R only occur in around 8% of the individual sites and for all three data sets, overall differences in R are more pronounced for this layer, mainly as a result of both the improved drainage formulation and the optimised data assimilation algorithm. Figure 3.3 shows maps of the difference in R against in situ measured surface soil moisture for the v3 and v2 data sets. Since most in situ sites are located in the CONUS, also a detailed view of the results over this area is presented (Figure 3.3b). As illustrated in these maps, the quality of the soil moisture data sets improves in most regions and for the majority of sites (blue colour). It could be argued

that in the Great Plains, the performance of GLEAM v3 is lower than for v2, yet only a limited number of sites are available in this area.

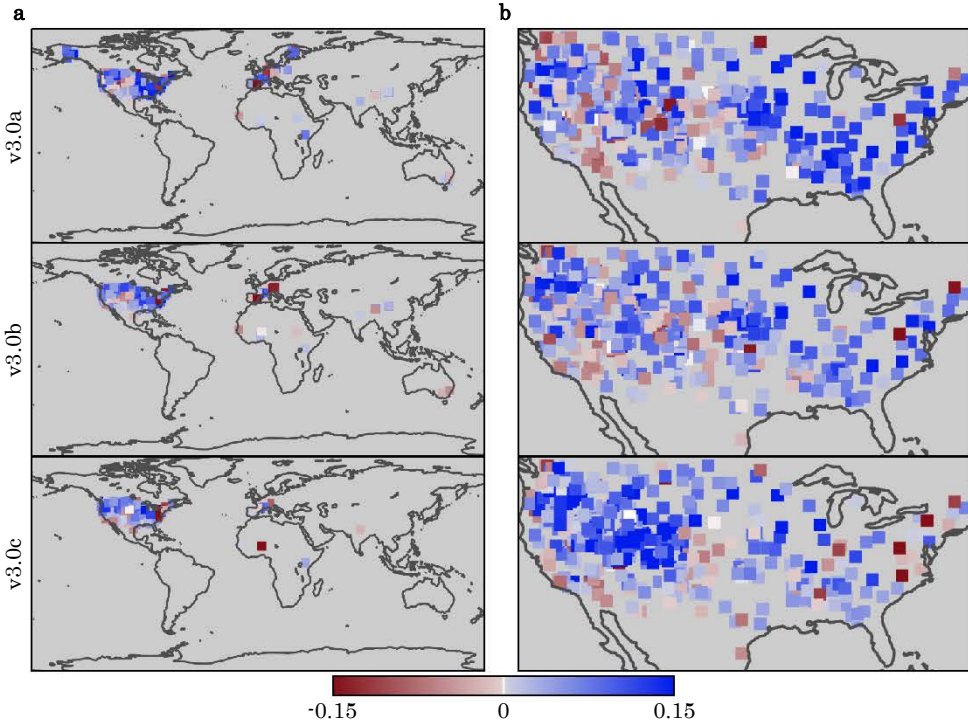


Figure 3.3: Maps indicating the quality difference between the v3 and v2 data sets of surface soil moisture presented as differences in Pearson correlation coefficient against in situ measurements (v3 minus v2). (a) Maps for the global domain and all in situ sites and (b) a detailed overview of the results for the CONUS.

Finally, to better evaluate the skill of GLEAM v3 to capture the effect of specific precipitation events on the estimated soil moisture – without the influence of the seasonal cycle – the correlation between the anomaly time series of GLEAM soil moisture and the anomaly time series of in situ soil moisture (R_{an}) are also calculated and reported in Table 3.3. Note that to calculate a robust climatology, only in situ sites with at least 5 years of data were used, resulting in a lower subset of stations and no anomaly-based evaluation for the v3.0c data set. As expected, correlations decay after the removal of the seasonal cycle, but remain in the range of 0.48–0.54 for the first layer and 0.43–0.49 for the second layer. In addition, results shown in Table 3.3 confirm the higher accuracy of the v3.0a soil moisture as compared to the v3.0b data set (significantly better correlations are obtained in 55% of the individual sites), and the higher performance of GLEAM v3 over the previous version (v2), with the number of significantly better correlations being similar as for the regular correlations (Table 3.2).

Table 3.3: Average anomaly correlations for different soil moisture data sets (v3.0a and b) and for the first two model layers ($w^{(1)}$ and $w^{(2)}$) against in situ measurements: R_{an} is the anomaly correlation and N is the number of sites included in the sample. The first part of the table reports the averaged statistics over all available sites and the entire study period, while the second part shows the same statistics for a common sample of sites, and an overlapping study period (2004–2015) for the two data sets. The same statistics for the data sets produced using GLEAM v2 are reported between brackets.

		Complete record		Overlap period	
		N	R_{an}	N	R_{an}
		(–)	(–)	(–)	(–)
v3.0a	$w^{(1)}$	515	0.54 (0.52)	455	0.55 (0.53)
	$w^{(2)}$	714	0.49 (0.45)	622	0.48 (0.45)
v3.0b	$w^{(1)}$	455	0.48 (0.47)	455	0.48 (0.48)
	$w^{(2)}$	623	0.43 (0.40)	622	0.42 (0.40)

Impact of the data assimilation system

Figure 3.4a shows the differences in Pearson correlation coefficient against the in situ measurements when data assimilation of satellite soil moisture is included in GLEAM v3 versus when it is not (i.e. model OL). As more than 75% of soil moisture validation sites are located in the CONUS, only the results for this region are shown here. For the v3.0a data set, the assimilation of the CCI soil moisture has a rather neutral to negative impact on the modelled soil moisture states of the first model layer. Generally, correlations are decreasing (red colour) after assimilation in very dry (e.g. West Coast of the CONUS) and forested regions (e.g. East Coast of the CONUS). This decrease is statistically significant in about 10% of the in situ soil moisture sites, while a neutral effect is obtained at the majority of the sites (89%). In regions of limited topography, dominated by sparse vegetation and strong seasonal variations in soil moisture (e.g. Great Plains), the quality of the modelled soil moisture is slightly improving (blue colour). For the v3.0b and v3.0c data sets, the assimilation of satellite-derived soil moisture (ESA CCI in v3.0b and SMOS L3 in v3.0c) has (in general) a more pronounced and positive impact (blue colour) on the modelled soil moisture, especially in areas such as the Great Plains. The latter can be expected given the higher quality of microwave soil moisture retrievals in regions with low vegetation cover (Dorigo *et al.*, 2015).

The negative impact of assimilating satellite observations of surface soil moisture in the v3.0a data set is partly explained by the high quality of the GLEAM OL soil moisture as compared to the quality of the satellite-based soil moisture data set (ESA CCI SM v2.3): correlations are significantly better for the OL in 73% of the individual sites. The high quality of the model OL in these regions is largely due to the accuracy of the MSWEP precipitation

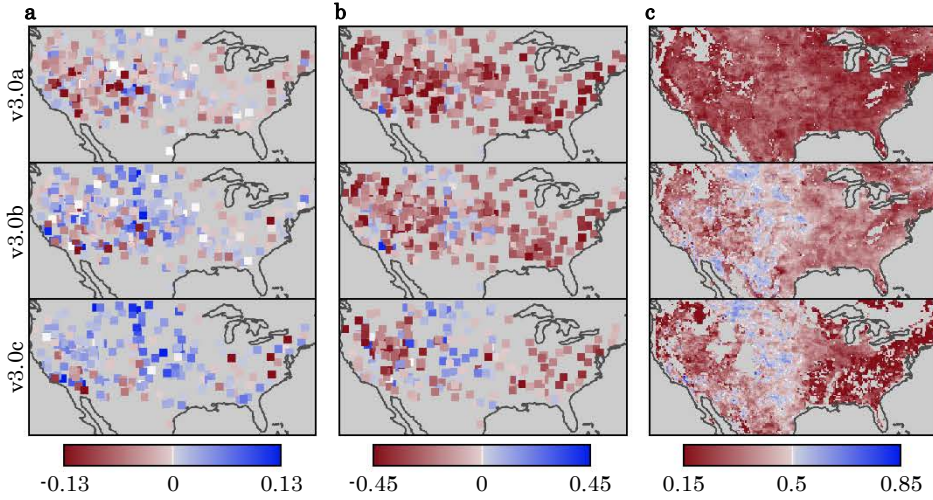


Figure 3.4: Impact of the data assimilation system in GLEAM v3 on the surface soil moisture for the CONUS. **(a)** Differences in Pearson correlation coefficient against in situ measurements between GLEAM v3 surface soil moisture with and without the assimilation of satellite-derived soil moisture. **(b)** Differences in Pearson correlation coefficient against in situ measurements between the satellite-derived soil moisture and GLEAM v3 without data assimilation. **(c)** Multi-annual average of the quality factor used in the data assimilation framework. The latter balances both the model and observation errors, with values above (below) 0.5 indicating a lower (higher) error in the observations relative to the OL.

forcing in the CONUS; this is illustrated in Figure 3.4b, where difference maps between the Pearson correlation coefficient against in situ measurements of the satellite soil moisture observations and the three OL data sets are shown. A clearly higher quality of the model OL in terms of correlations is highlighted for regions such as the East and West Coasts of the CONUS (red colour), and similar patterns are obtained for the ubRMSD (not shown). In those regions, the assimilation of satellite soil moisture may decrease model performance, especially in case of the v3.0a, where differences are more pronounced (see correspondence to Figure 3.4a). For the v3.0b and v3.0c data sets, the difference in quality between satellite soil moisture and OL is lower (the model OL is significantly better in 55% and 25% of the in situ sites for the v3.0b and v3.0c data sets, respectively). Moreover, the difference in correlations becomes even positive in regions with low vegetation (Figure 3.4b), pointing to the higher quality of the satellite-based soil moisture observations than that of the model estimates in those areas (e.g. the Great Plains). These maps point again to the above-mentioned lower quality of the v3.0b and v3.0c precipitation forcing in those regions (TRMM 3B42v7 compared to MSWEP). The subtle differences between the validation results for the v3.0b and v3.0c data sets relate to the

different quality of the CCI and SMOS soil moisture observations, respectively, bearing in mind the different study period and number of in situ stations used in their validation. Analogous results for anomaly time series are summarised in Figure 3.5 and point to the same conclusions as drawn from Figure 3.4.

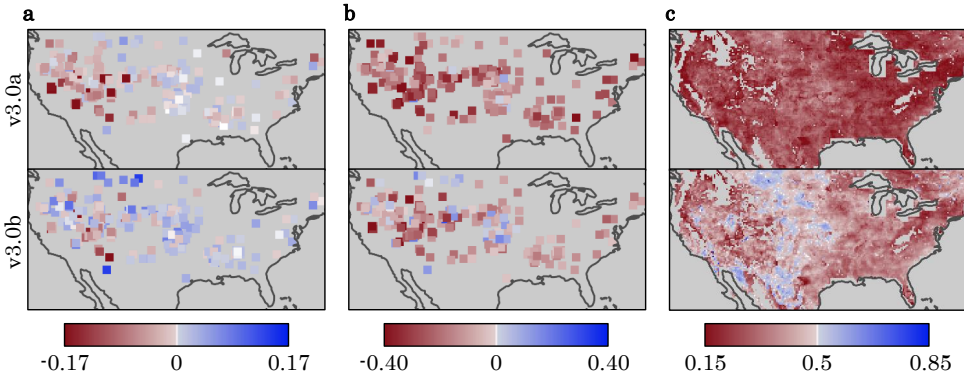


Figure 3.5: Impact of the data assimilation system in GLEAM v3 on the surface soil moisture for the CONUS. **(a)** Differences in Pearson correlation coefficient against anomalies of in situ measurements between GLEAM v3 surface soil moisture with and without the assimilation of satellite-derived soil moisture. **(b)** Differences in Pearson correlation coefficient against anomalies of in situ measurements between the satellite-derived soil moisture and GLEAM v3 without data assimilation. **(c)** Multi-annual average of the quality factor used in the data assimilation framework. The latter balances both the model and observation errors, with values above (below) 0.5 indicating a lower (higher) error in the observations relative to the OL.

Finally, it may be argued that differences in quality between the satellite-derived and modelled soil moisture should reflect in the TCA-based quality factor (γ) used in the data assimilation algorithm. The quality factor used in the Newtonian Nudging algorithm is estimated on a yearly basis by applying a TCA on the soil moisture anomalies of three independent data sets. Based on Equation 2.6 it can be seen that values of γ below (above) 0.5 point to a lower (higher) model error relative to the observation error. The multi-annual average quality factor for each of the three data sets is shown in Figures 3.4c and 3.5c. Spatial patterns in these maps agree well with the ones observed in Figures 3.4b and 3.5b, reflecting the ability of the TCA to capture the relative errors of modelled and observed surface soil moisture. Nonetheless, despite the overall low quality factors for the v3.0a data set (i.e. γ rarely exceeds 0.3) – which reflects the higher error of the observed soil moisture relative to the model OL – a decrease in quality is often observed when the ESA CCI soil moisture data set is assimilated into GLEAM v3.0a (see above discussion). As expected, the quality factors for the v3.0b and v3.0c data sets are higher and exceed 0.5 in some low-vegetated regions, indicating again the high quality of

the satellite-based soil moisture observations as compared to the model OL in these areas. In these regions, the impact of the data assimilation system is the highest, most probably due to strong seasonal variations in soil moisture and relatively low vegetation and thus higher quality soil moisture retrievals from satellites.

3.5.2 Validation of evaporation

Accuracy of evaporation estimates

Table 3.4 lists the validation statistics for the different evaporation data sets (Pearson correlation coefficients against the in situ data at all sites for the v3.0a, v3.0b, and v3.0c data sets, calculated for the entire validation period, are listed in Table A.2; Appendix A). In contrast to the results of the soil moisture validation exercise (Tables 3.2 and 3.3), differences between the three data sets are less pronounced. For the overlapping period 2011–2015 and the common sample of sites, an average correlation of approximately 0.78 and a similar ubRMSD of $0.71 \text{ mm} \cdot \text{day}^{-1}$ are obtained for all three data sets. In addition, differences are only significant at the 10% significance level at two in situ stations. Analogous statistical inferences for the validation of GLEAM v2 are shown between brackets and differ only slightly from the ones calculated for the data sets obtained using the new model version. At the majority of sites, no statistical significant difference in R is obtained. Figure 3.6a shows maps of the differences in Pearson correlation coefficient against the in situ measurements for the v3 and v2 data sets (Figure 3.6b shows the same but for correlations calculated at anomaly time series). Given the low number of in situ sites, no clear conclusions on geographical patterns can be drawn. Over continental Australia, GLEAM v3 performs generally better, except for the v3.0c data set, where for some sites a deterioration of the results is shown when compared to the corresponding v2c. However, as the validation data base for the latter contains a significantly lower number of measurements, due to the shorter time period, it may be less representative of the overall quality of the data set. Correlations for the anomaly time series are listed in Table 3.5 and confirm the above conclusions.

As an example, Figure 3.7 shows time series of GLEAM and in situ measured evaporation for two validation sites, i.e. US-Ne3 (Great Plains; Table A.2, Appendix A) in Figure 3.7a and AU-ASM (central Australia; Table A.2, Appendix A) in Figure 3.7b. While for the first site the performance of GLEAM v3 tends to be lower, statistics are improving for the second site with respect to the previous version of the model. Overall, time series show a good correspondence between model and in situ measurements. For US-Ne3, correlations drop from 0.82 (v2a) and 0.83 (v2b) to 0.78 (v3.0a) and 0.77 (v3.0b); contrary, for the SMOS-based data sets (v2c and v3.0c), correlations

Table 3.4: Average validation statistics for the different evaporation data sets (v3.0a–c) against in situ measurements: ubRMSD is the unbiased root mean squared difference, R is the Pearson correlation coefficient, and N is the number of sites included in the sample. The first part of the table reports the averaged statistics over all available sites and the entire study period, while the second part shows the same statistics for a common sample of sites, and an overlapping study period (2011–2015) for the three data sets. The same statistics for the data sets produced using GLEAM v2 are reported between brackets.

	Complete record			Overlap period		
	N	ubRMSD	R	N	ubRMSD	R
	(–)	(mm·day ^{–1})	(–)	(–)	(mm·day ^{–1})	(–)
v3.0a	91	0.72 (0.73)	0.81 (0.81)	41	0.71 (0.71)	0.79 (0.78)
v3.0b	63	0.75 (0.76)	0.80 (0.80)	41	0.71 (0.72)	0.78 (0.78)
v3.0c	44	0.74 (0.75)	0.78 (0.78)	41	0.71 (0.73)	0.78 (0.78)

Table 3.5: Average anomaly correlations for different evaporation data sets (v3.0a and b) against in situ measurements: R_{an} is the anomaly correlation and N is the number of sites included in the sample. The first part of the table reports the averaged statistics over all available sites and the entire study period, while the second part shows the same statistics for a common sample of sites, and an overlapping study period (2004–2015) for the two data sets. The same statistics for the data sets produced using GLEAM v2 are reported between brackets.

	Complete record		Overlap period	
	N	R_{an}	N	R_{an}
	(–)	(–)	(–)	(–)
v3.0a	53	0.42 (0.41)	34	0.41 (0.40)
v3.0b	35	0.46 (0.45)	34	0.43 (0.43)

increase from 0.73 to 0.76. Analogous differences are obtained in terms of ubRMSD. Despite the apparent decrease in quality for the v3 data sets, the time series shown for US-Ne3 illustrate that the estimates of evaporation are realistic and have no systematic errors. For AU-ASM, correlations consistently improve for all three data sets from 0.84 (v2a), 0.84 (v2b) and 0.78 (v2c) to 0.88 (v3.0a), 0.88 (v3.0b) and 0.84 (v3.0c), and similar improvements are obtained for the ubRMSD. Time series in Figure 3.7b show that the better results are mainly explained by the improved estimates of the evaporative flux during the dry season. For these periods, GLEAM v3 estimates lower volumes of evaporation, resulting in a closer agreement with the in situ measurements; although most of these differences are not statistically significant. This is mainly related to the new drainage formulation outlined in Section 3.2.1, which allows a faster dry-out during precipitation-free periods, leading to an increase in evaporative stress. Additionally, the new drainage algorithm also yields less extreme evaporation peaks after precipitation events, since the faster drainage

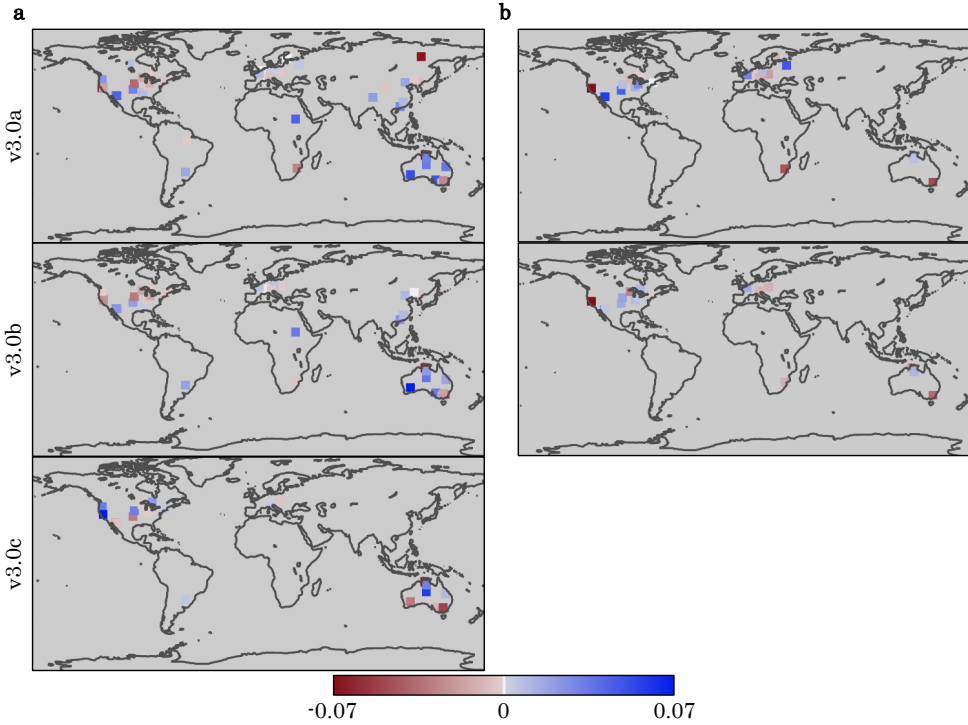


Figure 3.6: Quality difference between the v3 and v2 data sets of terrestrial evaporation presented as differences in Pearson correlation coefficient against in situ measurements (v3 minus v2). **(a)** Correlations calculated against the raw in situ measurements and **(b)** correlations calculated against anomalies.

implies that the soil profile requires stronger precipitation events to saturate. Results for AU-ASM indicate that these evaporation patterns are realistic under conditions of water stress, yet caution may be taken when extrapolating these findings to other climatic and ecological regimes.

Global magnitude and variability of terrestrial evaporation

Figure 3.8a presents the multi-annual total evaporation and its components from v3.0a, and their difference with respect to the v2a data set (Figure 3.8b). Analogous results are obtained for the v3.0b and v3.0c data sets, but are not shown for simplicity. As expected, the general climatic patterns of evaporation appear realistic, and are comparable to those reported by Miralles *et al.* (2016) and McCabe *et al.* (2016), based on a range of models and different forcing data. Differences in the annual totals between v3.0a and v2a amount to $100 \text{ mm} \cdot \text{year}^{-1}$ in several regions, with overall less evaporation in areas covered by short vegetation and more evaporation in deserts and tropical regions. The total global volume of evaporation (excluding inland water bodies) amounts

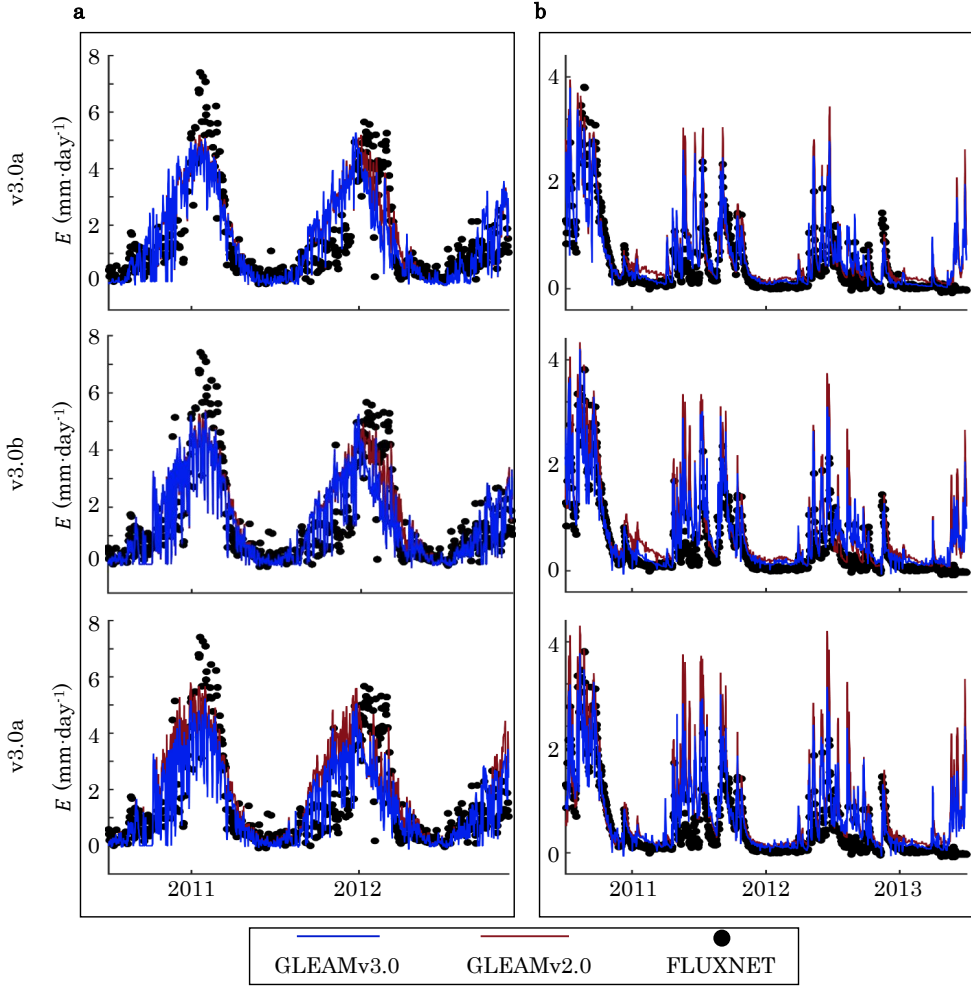


Figure 3.7: Time series of modelled evaporation (E). (a) Time series at site US-Ne3 and (b) AU-ASM.

to $66 \cdot 10^3 \text{ km}^3$ (v3.0a) versus the $68 \cdot 10^3 \text{ km}^3$ from the previous version (v2a); these numbers lay well within the previously reported range of values from independent sources – see e.g. Miralles *et al.* (2016) and references therein.

The remaining maps in Figure 3.8 show the partitioning of GLEAM evaporation into its different components, i.e. forest interception loss, transpiration, and bare soil evaporation. Note that for illustrative purposes only and to ease comparison to previous literature (Miralles *et al.*, 2016), the estimated sublimation is added to the bare soil flux and the evaporation from inland waters (open-water evaporation) is not considered here. Averaged over the entire land surface, approximately 74% of the total flux of water from land into the atmosphere is coming from transpiration, 15% comes from bare soil

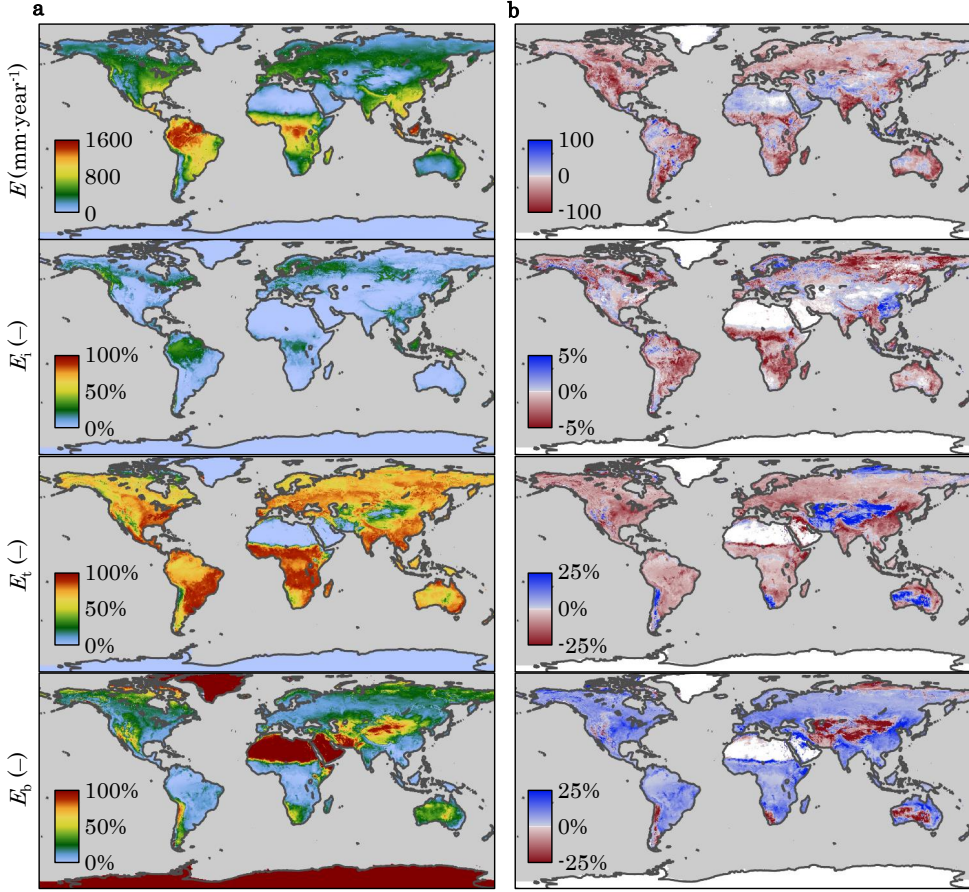


Figure 3.8: Global maps of terrestrial evaporation (E) and the partitioning in its different components, i.e. forest interception loss (E_i), transpiration (E_t), and bare soil evaporation (E_b). E is reported in $\text{mm}\cdot\text{year}^{-1}$, and its partitioning in percentages relative to this total. (a) Maps for the v3.0a data set of terrestrial evaporation, and (b) difference of the maps in (a) with their analogues from the v2a data set.

evaporation and about 11% is the result of interception loss; for the v2a data set, 80%, 8% and 12% are obtained, respectively. These discrepancies are also evidenced in the difference maps shown in Figure 3.8b. It can be seen that almost across the entire globe the bare soil evaporation is higher in the v3.0a data set; only for some drier regions such as the Namibian desert, central Australia, and parts of Chile, the bare soil evaporation has decreased. In contrast, transpiration typically increases in these areas. As shown, the total flux of interception loss is generally lower in the new version, except for some parts of Amazonia, eastern China, and the CONUS where a clear increase may be observed. All these differences are the result of the modified stress functions,

but – more importantly – of the new (high-resolution) land cover fractions used in GLEAM v3 which report an overall larger fraction of bare soil over the continents. The higher contribution of bare soil evaporation and the lower volumes of transpiration, especially in semi-arid regions like the Sahel, result in closer agreement with the partitioning obtained from other data sets (Miralles *et al.*, 2016; Good *et al.*, 2015; Schlesinger and Jasechko, 2014; Wang *et al.*, 2014). Nonetheless, Talsma *et al.* (2018a) and Miralles *et al.* (2016) recently raised awareness about the use of satellite-based evaporation algorithms to assess the contribution from different evaporation components, and suggested to avoid the use of any single model in isolation due to the large differences found in inter-model comparisons.

3.6 Conclusion

The available range of satellite-observable geophysical variables that relate to the process of evaporation – such as soil moisture, air temperature, and net radiation – is continuously growing and the quality of these data sets is constantly improving. As a result, models aiming at the accurate estimation of terrestrial evaporation from satellite observations need to be updated to optimally incorporate these new data. Concurrently, as our knowledge of the relevant physical processes advances based on new experimental evidence, these models should aim to increase their realism. With the overarching goal of improving our understanding of continental evaporation, a next version of GLEAM (v3) was presented in this chapter. Three major modifications are included: (1) a revised representation of the evaporative stress, (2) an optimised soil module, and (3) a new soil moisture data assimilation strategy. Using GLEAM v3, three novel data sets of root-zone soil moisture and terrestrial evaporation were presented. The first data set (v3.0a) spans the 36-year period 1980–2015, has a global coverage, and is produced using satellite-observed soil moisture, VOD, and snow-water equivalent, reanalysis air temperature and radiation, and a multi-source precipitation product. The remaining two data sets (v3.0b and v3.0c) are produced using satellite-based forcing only, with their difference being the use of SMOS-based VOD and soil moisture (v3.0c), as opposed to the corresponding CCI forcing (v3.0b). Both data sets are quasi-global (50°N–50°S) and span 2003–2015 for v3.0b, and 2011–2015 for v3.0c.

Results based on the validation of these three data sets against an extensive set of in situ measured evaporation and soil moisture point to a slightly higher quality of the v3.0a soil moisture data set as compared to the other two data sets, while the quality of the modelled evaporation is rather similar across all three. The higher accuracy of the v3.0a soil moisture is explained by the high quality of the MSWEP precipitation forcing over the regions where

soil moisture probes are located, compared to the satellite-based forcing in the v3.0b and v3.0c data sets. Results, however, might be biased given that the vast majority (i.e. more than 75%) of the in situ soil moisture sites are located in the CONUS, where gauge-based precipitation products are known to outperform satellite products (Beck *et al.*, 2017). Finally, the quality of the new v3 data sets is also compared to analogous data sets obtained using GLEAM v2. For the soil moisture, the modifications in GLEAM result in a consistent improvement across the vertical profile. These improvements mainly relate to the optimised drainage algorithm and the new data assimilation system, which allow a more realistic representation of the downward flux of water through the soil profile. The increased quality of the evaporation data is not revealed unambiguously by the in situ validation, likely hampered by the limited availability of validation sites. It is illustrated that, on average, the performance of GLEAM v3 is comparable to that of the former version. The partitioning of terrestrial evaporation into its different components shows an increase in bare soil evaporation almost in every continental region, while interception loss generally decreases, and transpiration increases for some dry regions such as the Namibian desert and central Australia. These results are related to the static data set describing the land cover fractions per grid cell, which is also updated in GLEAM v3. Based on the results in this study, it can be concluded that the modifications in GLEAM have led to a more realistic representation of physical processes and an overall increased quality of the data sets, particularly in the case of the root-zone soil moisture.

Within the frame of this dissertation, the data sets of terrestrial evaporation and root-zone soil moisture presented in this chapter have been made publicly available using www.GLEAM.eu (last visit: 18 November 2019) as gateway. These data sets are updated on an annual basis by forcing GLEAM with the latest version of the forcing data sets (Table 3.1) and extending the temporal coverage to near present. These data sets are widely-used by the scientific community as evidenced by more than 2200 registered users at www.GLEAM.eu (last visit: 18 November 2019), 160 citations of Martens *et al.* (2017)² at Web of Science, and 308 citations of the original paper by Miralles *et al.* (2011b)³. A non-exhaustive overview of studies using GLEAM is discussed in Section 7.2.

²This paper is marked as a “Hot Paper” by Web of Science meaning that the paper “received enough citations in January/February 2019 to place it in the top 0.1% of papers in the academic field of Geosciences”.

³Statistics were retrieved at 22 November 2019.

Estimating terrestrial evaporation at the regional scale using GLEAM at high resolution

In this chapter, GLEAM is for the first time applied at 100 m spatial resolution and daily time steps to provide estimates of terrestrial evaporation over The Netherlands, Flanders, and the west of Germany for the period 2013–2017. By making extensive use of microwave-based geophysical observations, data is available under all weather conditions, which is an indisputable advantage over more traditional methods – such as SEB-based methods forced with TIR-measurements of LST – to estimate terrestrial evaporation at these spatial scales. The data set is validated against eddy-covariance measurements from five sites, and in situ soil moisture measurements from 29 sensors across the study domain. The high-resolution GLEAM data set is also compared to estimates from the coarse-scale GLEAM, land evaporation from the Satellite Application Facility on Land Surface Analysis, and reference grass evaporation based on Makkink’s equation. This chapter is an edited version of the following scientific publication:

Martens, B., de Jeu, R.A.M., Verhoest, N.E.C., Schuurmans, H., Kleijer, J., Miralles, D.G., 2018. Towards estimating terrestrial evaporation at fields scales using GLEAM. *Remote Sensing* 10 (11), 1720.

4.1 Introduction

Traditional methods to estimate terrestrial evaporation with high spatial detail from remote sensing data typically use LST measurements in SEB-based models (Section 1.1.4). Nowadays, the use of LST – derived from TIR sensors onboard satellites (Anderson *et al.*, 2011), cubesats (McCabe *et al.*, 2017b), or drones (Hoffmann *et al.*, 2016) – in these algorithms allows estimating terrestrial evaporation at high spatial (up to 1 m using drones) and temporal resolutions (up to several minutes using geostationary imagery), with a limited need for ancillary data (Anderson *et al.*, 2011). However, TIR measurements are affected by clouds (Holmes *et al.*, 2016), restricting the estimation of terrestrial evaporation to times with optimal weather conditions (Anderson *et al.*, 2007). While estimates of LST from passive microwave observations might overcome this problem (Holmes *et al.*, 2018, 2016), they suffer from a substantially coarser native spatial resolution (several kilometres). In addition to these weather-related issues, SEB models target the accurate estimation of the sensible heat flux, relying on assumptions regarding the vertical temperature gradient, and the aerodynamic conductance of the atmosphere. Subsequently, they calculate the surface latent heat flux as the residual of the SEB, propagating all errors into the estimate of the flux (Kalma *et al.*, 2008; Su, 2002; Bastiaanssen *et al.*, 1998; Kustas, 1990).

Alternative methods to derive terrestrial evaporation directly target the flux using process-based algorithms (Section 1.1.4). However, most of them have been originally designed for global-scale applications (Zhang *et al.*, 2016b; Miralles *et al.*, 2011b; Zhang *et al.*, 2010; Fisher *et al.*, 2008; Mu *et al.*, 2007). GLEAM is such a model; however, the application of GLEAM for local water management or agricultural planning has been hindered by its spatial resolution, resulting from the coarse-scale inputs typically used to force the model (Chapters 2 and 3). Nonetheless, the algorithm is in principle applicable at finer resolutions if the required forcing data are available.

Recent progress in the field of Earth observation has resulted in a plethora of satellite-based observations spanning multiple spatial and temporal scales (McCabe *et al.*, 2017a). Also in the microwave domain, efforts to combine measurements from different sensors and to improve retrieval algorithms (de Jeu *et al.*, 2017; van der Schalie *et al.*, 2015b,a) have resulted in the availability of microwave-based geophysical parameters at field scales (de Jeu *et al.*, 2017). These advances enable the estimation of terrestrial evaporation using GLEAM at similar spatial scales.

In this chapter, GLEAM is forced using novel, all-weather, high-resolution (100 m) microwave data over The Netherlands, Flanders and the west of Germany to assess the capability of the model to estimate terrestrial evaporation at these scales. The high-resolution estimates of terrestrial evaporation are validated against in situ measurements from five eddy-covariance towers within

the study domain. In addition, the surface soil moisture estimates from GLEAM are also validated using in situ measurements from 29 soil moisture sensors. The quality of the high-resolution terrestrial evaporation data set is further compared to similar data sets available over the study domain. Finally, the spatial patterns of terrestrial evaporation are evaluated, and the response of evaporation to the summer drought in 2013 is discussed. As GLEAM has been designed to estimate terrestrial evaporation at the global scale and relatively coarse spatial resolution (± 25 km), this study will provide insights on the applicability of the model assumptions and structure at much finer resolution, which will foster the estimation of terrestrial evaporation at resolutions useful for local water resources management and agriculture. The chapter is organised as follows: Section 4.2 presents the forcing and validation data used in this chapter, Section 4.4 discusses the main results of this study, including a temporal and spatial evaluation of the high-resolution estimates from GLEAM and a comparison to alternative data sets, and Section 4.5 summarises the main findings of this study.

4.2 Data

4.2.1 Input data sets

Table 4.1 lists the data sets used in this study to force GLEAM. All variables are processed over The Netherlands, Flanders, and the west of Germany and are linearly resampled to a 100 m spatial grid and (when necessary) aggregated to a daily temporal resolution. Except for the soil properties (used to parameterise the soil-water balance model in GLEAM; Section 3.2.1), and the precipitation data set, all forcing variables are obtained from satellite-based measurements. Note that atmospheric forcing variables (such as incoming radiation and precipitation) come originally at coarser spatial resolution, but because atmospheric forcing is more spatially uniform than the (heterogeneous) land surface properties, the use of 100 m as target resolution appears justified.

Aiming at the most accurate calculation of the available energy at the surface, radiation components from different satellite-based data sets are combined. Incoming shortwave and longwave surface radiation fluxes are retrieved from measurements of the Spinning Enhanced Visible and Infrared Imager (SEVIRI) onboard the Meteosat Second Generation (MSG) satellite, and are obtained from the European organisation for METeorological SATellites (EUMETSAT) Satellite Application Facility on Land Surface Analysis (LSA-SAF; Trigo *et al.*, 2011). The native spatial resolution of the SEVIRI instrument is 3.1 km at nadir, but reduces towards approximately 5 km over Europe. Albedo – required to estimate the reflected shortwave radiation at the surface – is sourced from measurements of the MODIS instruments onboard Terra and Aqua. Here, the 16-day MCD43A3 albedo product (Schaaf and Wang, 2015) at 500 m spatial

resolution is used, which is linearly resampled to a daily time interval. Finally, the emitted longwave radiation flux at the surface is estimated using land surface emissivity from LSA-SAF (Trigo *et al.*, 2011) and microwave-based estimates of LST at 100 m spatial resolution from VanderSat (de Jeu *et al.*, 2017). To obtain consistent radiation fluxes, each flux is individually scaled towards its coarse-scale analogue obtained from measurements of CERES onboard Terra (Wielicki, 1996). The scaling involves a multiplicative bias-correction at the 1° spatial resolution of CERES, preserving the higher resolution spatial features of the underlying data sets (Appendix B).

Precipitation is obtained from a network of five ground-based, C-band Doppler radars located in The Netherlands (operated by the Royal Meteorological Institute of The Netherlands, KNMI) and Germany (operated by the German Weather Service). Individual radar images are first merged, and subsequently corrected using in situ rain gauge measurements (Royal Haskoning DHV and Nelen en Schuurmans, 2013). The final daily data set is curated by Royal Haskoning DHV (<https://www.royalhaskoningdhv.com/>; last visit: 16 November 2019) and is available at a 1 km spatial resolution.

VOD, surface soil moisture, and LST are retrieved by the LPRM (van der Schalie *et al.*, 2015b,a; Owe *et al.*, 2008) on downscaled measurements of the AMSR-2 instrument onboard the GCOM-W1 satellite. The data are available at a daily time interval and 100 m spatial resolution (de Jeu *et al.*, 2017). Because GLEAM uses TCA to compute the uncertainties in the microwave-based soil moisture that is assimilated (Section 3.2.2), a third independent data set of soil moisture is also required. Here, the soil-water index calculated from measurements of the Advanced SCATterometer (ASCAT) onboard Metop A and B from Albergel *et al.* (2008) is adopted. Note that given the daily availability of microwave surface soil moisture observations in this study, the nudging factor (K , Equation 3.2) in the data assimilation system is decreased from the value of 1 used in Chapters 2 and 3 to a value of 0.25. The latter avoids that the model is nudged too strongly towards the observations and thus relaxes the dependence of the model estimates on the microwave observations of surface soil moisture (Stauffer and Seaman, 1990).

The static data sets of land cover fractions and lightning frequency are the same as in Section 3.3.1, except that they are processed at the finest resolution. Contrary, soil properties are obtained from the SoilGrids250m data set, which is based on a spatial interpolation using an ensemble of machine learning methods trained on a global data set of in situ soil profiles and satellite-derived input data sets (Hengl *et al.*, 2017).

Table 4.1: List of the selected data sets used to produce the forcing for GLEAM-HR together with an indication of the type of data, their approximate native spatial and temporal resolution, and their reference.

Variable	Data set	Type	Resolution		References
			Spatial	Temporal	
Radiation	CERES L3SYN1DEG	Satellite	110 km	3 hours	Doeling (2017)
Emissivity	Meteosat LSA-SAF	Satellite	3.1 km	1 day	Trigo <i>et al.</i> (2011)
	Meteosat LSA-SAF	Satellite	3.1 km	1 day	Trigo <i>et al.</i> (2011)
Albedo	MODIS MCD43A3	Satellite	500 m	16 day	Schaaf and Wang (2015)
LST	VanderSat LST-I00	Satellite	100 m	1 day	de Jeu <i>et al.</i> (2017)
Precipitation	Nationale Regenradar	Ground radar	1 km	5 min	RH2013
VOD	VanderSat VOD-C1N-100	Satellite	100 m	1 day	de Jeu <i>et al.</i> (2017)
Soil moisture	VanderSat SM-C1N-100-SWI-T10	Satellite	100 m	1 day	de Jeu <i>et al.</i> (2017)
	ASCAT-SWI	Satellite	10 km	1 day	Albergel <i>et al.</i> (2008)
Cover fractions	MODIS MOD44B	Satellite	250 m	1 year	Dimiceli <i>et al.</i> (2015a)
Soil properties	SoilGrids250m	Merge	250 m	static	Hengl <i>et al.</i> (2017)
Lightning	LIS/OTD	Satellite	5 km	1 month	Cecil <i>et al.</i> (2014)

4.2.2 Validation data sets

In situ soil moisture and evaporation

Table A.3 (Appendix A) lists the eddy-covariance sites used in this chapter. Note that in situ measurements are only processed for the period 2013–2017, as 2012 is used to spin up GLEAM. Measurements from NL-Ca1 are downloaded from the Cabauw Experimental Site for Atmospheric Research (CESAR) web portal, while data from DE-RuR originates from the TERrestrial EnviroNmental Observatories (TERENO) data infrastructure. Data from DE-RuS are sourced from the European Fluxes data base cluster, and measurements from BE-Bra and NL-Loo are acquired from the FLUXNET 2015 data set. In situ measurements of surface soil moisture (i.e. sensors installed at a maximum depth of 10 cm, corresponding to the lower level of the first soil layer in GLEAM; Section 2.2.1) are obtained from the data base of the ISMN (Dorigo *et al.*, 2013, 2011), and the regional soil moisture network in the Raam catchment (Benninga *et al.*, 2018). All in situ data are processed as in Section 3.3.2.

Aiming at a robust validation, only stations reporting a minimum of 150 measurements after masking are considered in this study, resulting in a validation data set with measurements from five (corresponding to roughly 15 site years) eddy-covariance towers (Table A.3, Appendix A), and 29 surface soil moisture sensors. As in Section 3.3.2, measurements from sensors falling within the same 100 m model grid cell are not averaged to avoid potential problems with data gaps and biases between in situ sensors. Figure 4.1 shows the locations of the in situ sites within the bounding box of the study domain, with the multi-annual yearly normalised difference vegetation index from LandSat 8 as a background. Eddy-covariance sites span different vegetation types and are well-distributed across the study domain, as shown in Figure 4.1. Soil moisture validation sites are clustered in the Eifel area in west Germany, and the Raam catchment in the east of The Netherlands. The latter is an intensively-measured, medium-scale 223 km² catchment where data from 14 soil moisture sensors are available (Benninga *et al.*, 2018). Also note that at DE-RuR, DE-RuS, and NL-Loo, both measurements of surface soil moisture and terrestrial evaporation are available.

Gridded evaporation

The high-resolution GLEAM evaporation data (hereafter referred to as GLEAM-HR) are also compared against the LSA-SAF (Trigo *et al.*, 2011), GLEAM v3.2b¹, and Makkink (<https://data.knmi.nl/>; last visit: 22 November 2019) daily evaporation products.

¹This data set is an updated version of the v3.0b data set presented in Chapter 3. Differences include minor algorithmic updates in GLEAM and new versions of the forcing data sets.

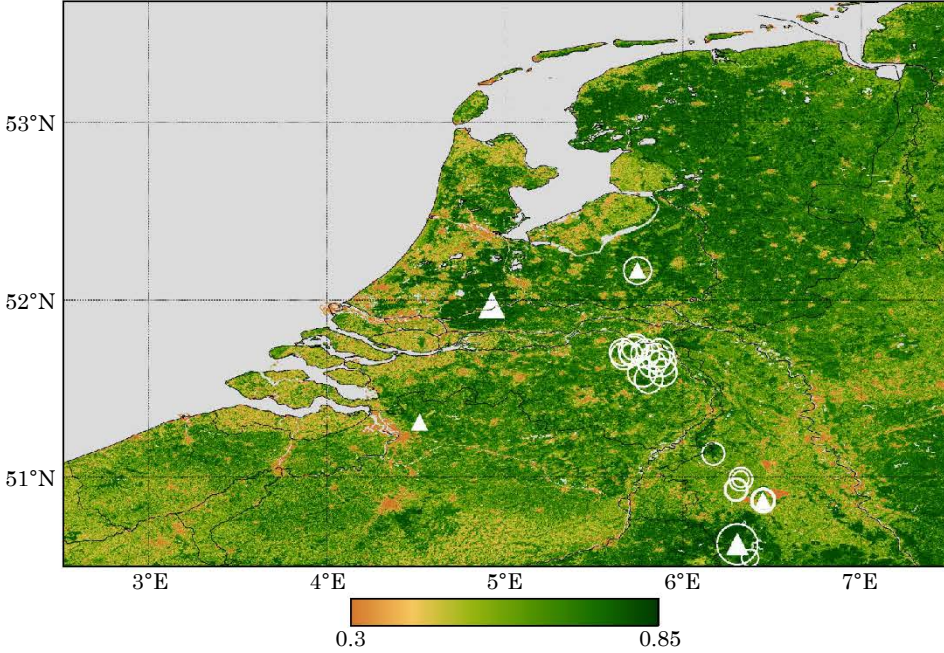


Figure 4.1: Multi-annual (2013–2017) yearly normalised difference vegetation index from Landsat 8 over the study domain with indication of in situ soil moisture sites (open circles) and eddy-covariance towers (triangles). The outline of the symbols is linearly proportional to the length of the data record at the sites.

LSA-SAF is obtained from forcing a physically-based soil vegetation atmosphere model with inputs derived from MSG-SEVIRI and meteorological forecasts from ECMWF (Ghilain *et al.*, 2011). Similar to GLEAM, the algorithm first estimates evaporation for several sub-pixel land cover units – characterised using the ECOCLIMAP data set (Masson *et al.*, 2003) – and aggregates the resulting estimates to the pixel level. The model is parameterised using look-up tables and the ECOCLIMAP data set. Estimates are available at the native resolution of the MSG-SEVIRI instrument, which is approximately 5 km over western Europe. KNMI provides a daily evaporation product for The Netherlands by interpolating reference grass evaporation estimated from meteorological measurements at 32 sites using the Makkink equation (De Bruin, 1981; Makkink, 1957). The latter is a radiation-based approach and only provides an estimate of terrestrial evaporation for a well-watered reference grass, essentially ignoring the actual surface control on terrestrial evaporation (i.e. impact of environmental stressors and the presence of the actual vegetation). The estimates are then interpolated using a thin plate spline method over a 10 km grid.

4.3 Experimental setup

In this chapter, GLEAM v3 is run over The Netherlands, Flanders, and the west of Germany at 100 m spatial resolution and at a daily time step for the period 2012–2017 (GLEAM-HR). As in Section 2.4, the soil moisture of each model layer in GLEAM is initialised as the average of the wilting point and field capacity in the grid cell, and the first year of the study period is used as a spin-up, hence it will not be considered in the evaluation of the model.

Daily surface soil moisture and terrestrial evaporation from GLEAM are evaluated against in situ measurements (Section 4.2.2) using the Pearson correlation coefficient, Mean Difference (MD), Mean Absolute Difference (MAD), and unbiased MAD (ubMAD) as primary validation statistics. The estimates of GLEAM-HR are also compared against alternative data sets (Section 4.2.2) and the OL of GLEAM-HR is compared against the run with data assimilation to assess the impact of the latter². Finally, a time series analysis is conducted, the spatial patterns across the study domain are analysed and compared against alternative data sets (Section 4.2.2), and the response of terrestrial evaporation to anomalously dry conditions is analysed.

4.4 Results and discussion

4.4.1 Validation of soil moisture

Given the relatively high volumes of rainfall, water availability is generally not limiting the evaporative flux in the study domain (Jacobs *et al.*, 2010; Jacobs and De Bruin, 1998; De Bruin, 1981). Nevertheless, a validation of the soil moisture estimates from GLEAM-HR against in situ measurements serves the purpose of identifying potential issues with regards to the input data and tests the validity of the algorithm at high resolutions. Figure 4.2 shows violin plots of the validation statistics calculated at the 29 in situ sites with surface soil moisture measurements. Statistics are shown for the microwave observations that are assimilated in GLEAM-HR (Table 4.1), GLEAM-HR without data assimilation (i.e. the OL), GLEAM-HR with assimilation of microwave soil moisture, and the coarse-scale GLEAM v3.2b data set.

Soil moisture estimates from GLEAM-HR compare reasonably well against in situ measurements, with a median R of 0.76, and values below 0.64 at only 7 of the in situ sites (Figure 4.2a). The estimates are close to unbiased (Figure 4.2b), but show a small tendency to overestimate the in situ data. The MAD roughly varies between 0.03 and 0.13 $\text{m}^3 \cdot \text{m}^{-3}$ (95%-interval), with a median of 0.07 $\text{m}^3 \cdot \text{m}^{-3}$ (Figure 4.2c). Part of the latter value is attributed

²Note that GLEAM-HR refers to the run with the assimilation of surface soil moisture, unless specified differently.

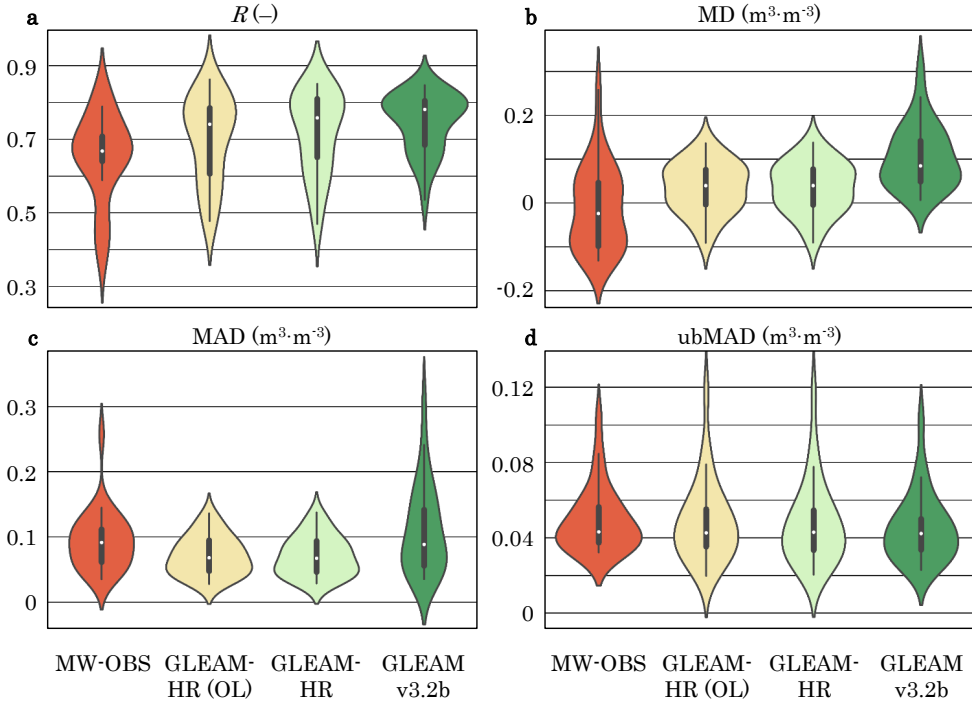


Figure 4.2: Violin plots of the validation statistics of surface soil moisture from microwave observations (MW-OBS), GLEAM-HR without data assimilation (OL), GLEAM-HR, and GLEAM v3.2b. Individual statistics are calculated for 29 soil moisture sensors and the violin plots represent the distribution of the statistics with indication of the median (white dot), interquartile range (thick line), and 95% interval (thin line). **(a)** Violin plots for the Pearson correlation coefficient (R), **(b)** Mean Difference (MD, in situ as a reference), **(c)** Mean Absolute Difference (MAD), and **(d)** unbiased MAD (ubMAD).

to the bias, as the ubMAD has a median close to $0.04 \text{ m}^3 \cdot \text{m}^{-3}$ (Figure 4.2d), which is below the threshold of $0.05 \text{ m}^3 \cdot \text{m}^{-3}$ that is often considered as the target accuracy for satellite-based soil moisture data sets (Chan *et al.*, 2018; Kerr *et al.*, 2012).

The microwave soil moisture observations generally show lower correlations (median of 0.67, Figure 4.2a) than the OL of GLEAM-HR, but comparable ubMAD (median of $0.04 \text{ m}^3 \cdot \text{m}^{-3}$, Figure 4.2d). In addition, the bias of the microwave observations is close to zero, with a tendency to underestimate the in situ soil moisture (Figure 4.2b). Assimilating the microwave observations in GLEAM-HR has a small but positive impact on the estimates of surface soil moisture: comparing the violin plots of GLEAM-HR against the ones for the OL of GLEAM-HR reveals an overall increase in R (upward shift of the

distribution, Figure 4.2a). Note that the MD of the OL and GLEAM-HR are the same (Figure 4.2b), as the data assimilation includes a scaling of the microwave observations towards the soil moisture estimates of the OL (Section 3.2.2). The impact of the data assimilation system on the MAD and ubMAD is less clear, but slightly positive (Figures 4.2c and d). The relatively simple data assimilation algorithm implemented in GLEAM-HR is thus able to extract valuable information from the microwave observations, and to increase the overall quality of the GLEAM-HR soil moisture estimates.

Temporal statistics in Figure 4.2 reveal that the soil moisture dynamics from the global GLEAM v3.2b are relatively reliable, despite their coarser spatial resolution. Figure 4.2a shows that both the median and third quartile of the R -distribution are rather similar for GLEAM-HR and GLEAM v3.2b. However, the Pearson correlation coefficient at a couple of sites is lower for GLEAM-HR, while for GLEAM v3.2b the correlation coefficients are consistently concentrated around their median value of 0.78. The MD (Figure 4.2b) of GLEAM-HR is considerably lower than that of GLEAM v3.2b, also resulting in lower values of the MAD (Figure 4.2c), while the ubMAD is similar for both data sets (Figure 4.2d). The lower bias for GLEAM-HR can be attributed to the added realism of the soil properties used in GLEAM-HR that set the range of absolute soil moisture values. Differences in R and the ubMAD reflect discrepancies in the dynamic forcing used in both. Uncertainties in net radiation and, to the largest extent, precipitation control the temporal variability of the surface soil moisture estimates from GLEAM-HR and its agreement against in situ measurements.

Despite that the ground-based radar composite used in this study (Table 4.1) covers the west of Germany and Flanders, the quality over these regions is lower due to the lower number of in situ rain gauges in these areas available to correct the radar retrievals (note that this effect might also occur along the coast of The Netherlands, since only inland gauges are used here; Royal Haskoning DHV and Nelen en Schuurmans, 2013). Only considering soil moisture validation sites in The Netherlands has a clear and positive impact on the validation statistics of GLEAM-HR (Supplementary Figure C.1, Appendix C.1), as most sites with poor validation statistics are removed from the sample. In addition, both the median and third quartile of the R -distribution are higher than the ones from GLEAM v3.2b at the same sample of sites, while the first quartile of the distribution still remains slightly lower (Supplementary Figure C.1a, Appendix C.1). Conclusions in terms of MD, MAD, and ubMAD remain similar (Supplementary Figures C.1b–d, Appendix C.1).

It should be emphasised that the results for this evaluation may not provide an unbiased assessment of the quality of soil moisture over the entire domain, due to the high concentration of in situ sensors in the Raam catchment (Figure 4.1), while only a limited number of sensors is available in other parts

of the study area with different soil properties, land cover, and atmospheric forcing. Given the strong spatial variability of parameters dominating the temporal dynamics (and spatial patterns) of surface soil moisture, it is thus difficult to generalise these results to the whole study area.

4.4.2 Validation of evaporation

Temporal evaluation

Figure 4.3 shows diamond plots of the validation statistics for the estimates of terrestrial evaporation from GLEAM-HR, the OL of GLEAM-HR, the coarse-scale GLEAM v3.2b, LSA-SAF, and the Makkink data set at each eddy-covariance site. Estimates from GLEAM-HR compare well with in situ measurements of evaporation, with a median correlation coefficient of 0.78 across all five sites. On average, a slight negative bias is observed, except for BE-Bra and NL-Loo, where GLEAM-HR tends to overestimate evaporation. The ubMAD ranges between $0.37 \text{ mm}\cdot\text{day}^{-1}$ at NL-Ca1 and $0.77 \text{ mm}\cdot\text{day}^{-1}$ at NL-Loo.

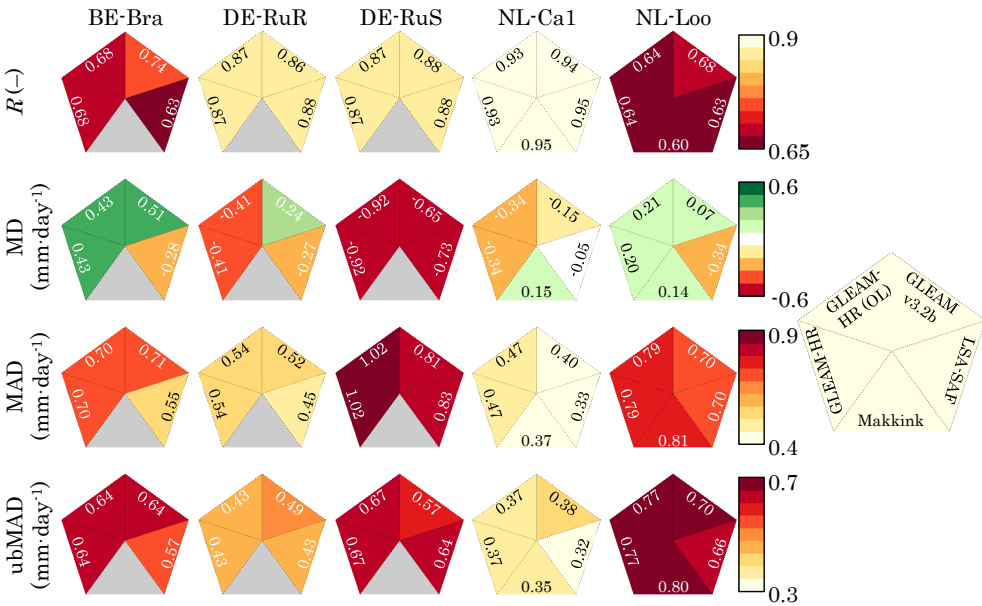


Figure 4.3: Validation statistics of terrestrial evaporation from GLEAM-HR, GLEAM-HR without data assimilation (OL), GLEAM v3.2b, LSA-SAF, and the Makkink data set. Validation statistics are calculated at five eddy-covariance sites and include the Pearson correlation coefficient (R), Mean Difference (MD, in situ as a reference), Mean Absolute Difference (MAD), and unbiased MAD (ubMAD). Grey indicates no data. For all plots, lighter colours represent relative better statistics.

The impact of soil moisture data assimilation on the estimates of evaporation from GLEAM-HR is negligible due to the relatively wet climate in the study domain, and consequently, the low control of soil-water availability on terrestrial evaporation (Jacobs *et al.*, 2010; Jacobs and De Bruin, 1998; De Bruin, 1981). Averaged over the five eddy-covariance sites, surface soil moisture from GLEAM-HR only drops below the critical soil moisture – i.e. the value where evaporation starts to be limited by soil-water availability in GLEAM (Section 3.2.3) – at 11% of the days in the study period. Note that surface soil moisture below the critical value does not necessarily imply that potential evaporation is constrained by water availability, as deeper soil layers might still provide access to water as described in Section 3.2.3. As such, the actual percentage of time that the evaporative flux is limited by the water availability in GLEAM-HR is lower than 11%, indicating the poor control of soil water availability over evaporation in the study domain.

In general, differences between temporal validation statistics across data sets are low. GLEAM v3.2b shows slightly higher values for R at BE-Bra and NL-Loo, but worse ubMAD at DE-RuR and NL-Ca1 than GLEAM-HR. LSA-SAF is the only data set consistently underestimating the in situ measurements, but shows similar values for the other statistics. Contrary, validation statistics differ substantially between the five in situ sites. At DE-RuR, DE-RuS, and NL-Ca1, all products perform considerably better than at the other two sites, with correlation coefficients reaching 0.9 at the sites in Germany, and 0.95 at NL-Ca1, indicative of the strong temporal agreement between the products and the in situ measurements. Similar conclusions may be drawn for the other statistics, except at DE-RuS, where the MD and MAD are also the highest across all sites, and for all products. At BE-Bra and NL-Loo, all products perform relatively worse, with values for R between 0.6 and 0.7, depending on the data set and site. Note again that eddy-covariance measurements tend to underestimate the latent heat flux and that the energy balance is generally not closed due to sub-optimal atmospheric conditions for eddy-covariance calculations at certain times, mismatch in the spatial footprint of different sensors at the tower, and poor characterisation of the soil heat flux (Section 1.1.3). As such, the consistently worse performance by all models at certain sites might reflect uncertainty in the in situ data as well. In the case of BE-Bra, the site is in the close proximity of an urban area; the impact of this aspect on the measurements, and the fact that none of the algorithms considered here parameterises specifically urban areas, may affect validation results as well.

At NL-Ca1 and NL-Loo, the Makkink data set is also evaluated (note that the Makkink data set is only available over The Netherlands as described in Section 4.2.2). Correlation coefficients of 0.95 and 0.6 are obtained for NL-Ca1 and NL-Loo, respectively; similar to the other data sets. However, the data set

consistently overestimates terrestrial evaporation at both sites, as the Makkink equation only considers the atmospheric demand for water over a reference grass, and does not account for any land surface control over the flux. The high correlation indicates the strong temporal agreement between potential and actual evaporation over The Netherlands, which has already been highlighted by Jacobs *et al.* (2010) and Jacobs and De Bruin (1998). However, the bias demonstrates the need for a proper (seasonally-dependent) crop coefficient to account for the land surface control and thus to convert potential into actual evaporation (Jacobs *et al.*, 2010; Jacobs and De Bruin, 1998).

Figure 4.4 shows time series of GLEAM-HR, GLEAM v3.2b, LSA-SAF, and the Makkink data set at NL-Ca1 (Figure 4.4a) and NL-Loo (Figure 4.4b). These time series show that all products are able to capture the seasonal cycle of terrestrial evaporation at both sites. As expected, differences at NL-Ca1 are small, and all products closely follow the in situ measurements. At NL-Loo, more explicit differences are found, especially during winter time where GLEAM-HR and GLEAM v3.2b show both larger variability and absolute values of terrestrial evaporation. This might be explained by the explicit consideration of rainfall interception loss in the algorithm, which becomes relatively more important during winter given the low volumes of transpiration and bare soil evaporation. Note that this can also be seen at NL-Ca1, although less clear. Also in summer 2013, clear differences between the products can be found at NL-Loo, which can be related to the different sensitivities of the algorithms to decreasing soil-water availability (see further).

Spatial evaluation

Figure 4.5a shows the multi-annual (2013–2017) mean of terrestrial evaporation from GLEAM-HR, GLEAM v3.2b, LSA-SAF, and the Makkink product, and the difference of each with the multi-product ensemble mean (Figure 4.5b). Note that the study area is limited to The Netherlands here because of the lower quality of the radar rainfall in GLEAM-HR outside the country (Section 4.4.1), and the fact that the Makkink product is only available for this area. All data sets show substantial differences, with GLEAM-HR and GLEAM v3.2b typically bounded by the low values from LSA-SAF, and the high values from the Makkink data set. The mean evaporation over The Netherlands amounts to 494, 569, 437, and 602 mm·year⁻¹ for GLEAM-HR, GLEAM v3.2b, LSA-SAF, and the Makkink product, respectively. Note that the relatively higher values for the Makkink data set are due to the fact that it represents reference grass evaporation rather than actual evaporation (Makkink, 1957), while the lower values in LSA-SAF might relate to the non-specific consideration of rainfall interception loss (Ghilain *et al.*, 2011), which represents a substantial fraction of the total flux in forested areas (Zhang *et al.*, 2016b; Miralles *et al.*, 2011a).

Despite similar temporal statistics, Figure 4.5a shows that all data sets

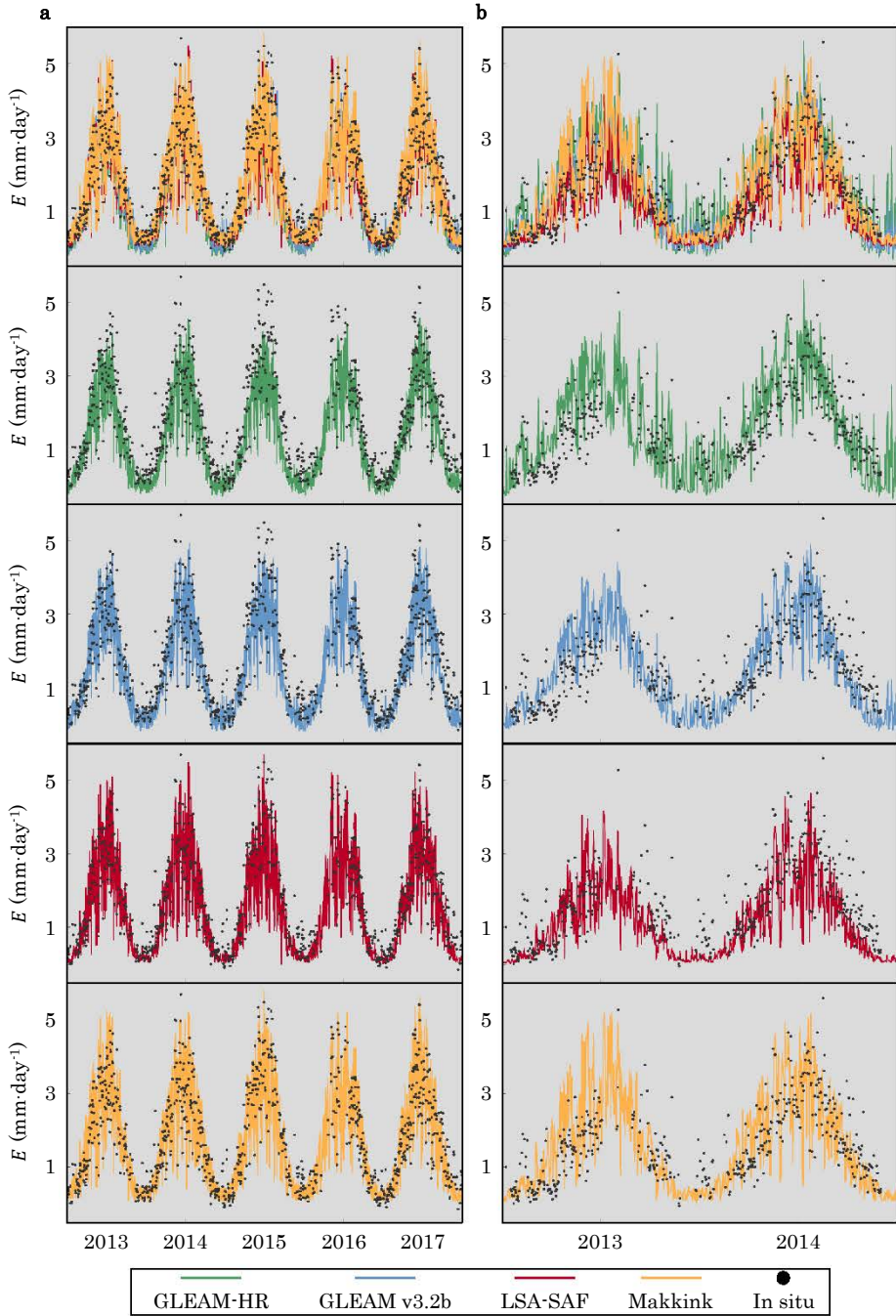


Figure 4.4: Time series of modelled and in situ measured terrestrial evaporation (E).
 (a) Time series at site NL-Ca1 and (b) NL-Loo.

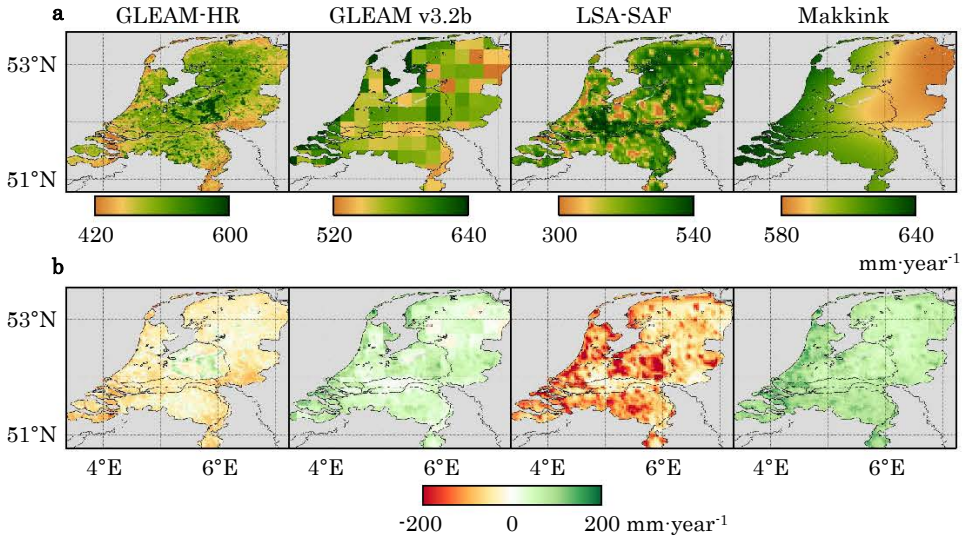


Figure 4.5: Maps of terrestrial evaporation for The Netherlands. **(a)** Multi-annual yearly terrestrial evaporation from GLEAM-HR, GLEAM v3.2b, LSA-SAF, and Makkink, and **(b)** their difference with the multi-product ensemble mean.

present substantially different spatial patterns. The highest spatial detail is reflected by GLEAM-HR. Contrary, the Makkink data set shows a smooth spatial pattern due to its spline interpolation based on a limited number of stations, and its high dependency on total incoming radiation (Makkink, 1957), reflected by a very gradual increase towards the southwest. However, spatial gradients in the Makkink data set are small as compared to the other data sets (note the different colour range used in Figure 4.5a).

Although obtained using the same algorithm, GLEAM v3.2b and GLEAM-HR show substantial differences in their spatial detail and magnitudes. Obviously, the higher spatial detail in GLEAM-HR can be attributed to the high-resolution forcing and more detailed parameterisation of the land surface. Given that the radiation forcing of GLEAM-HR is bias-corrected using the GLEAM v3.2b radiation forcing (Section 4.2.1 and Appendix B), differences in magnitude are most probably due to the rainfall forcing, mainly affecting the interception loss volume in the study domain. Note that given the low evaporative stress throughout the year, the effect of the rainfall forcing on the dynamics of the other evaporation components is negligible.

The overall patterns in GLEAM-HR and LSA-SAF are substantially different as well (Figure 4.5a). Both data sets agree on the lower values near the coast, which relate to the presence of large urban areas like Rotterdam, The Hague, and Amsterdam (Supplementary Figure C.2a, Appendix C.1). While urban areas are not explicitly modelled in any of the algorithms, they are associated

with a large fraction of bare soil and high LST, which yields low evaporation estimates. In case of LSA-SAF, the low values for most cities in The Netherlands (Supplementary Figure C.2a, Appendix C.1) are more apparent. The maximum annual evaporation is reported by LSA-SAF at approximately 52°N–5°E in the Green Heart of The Netherlands, a large vegetated area dominated by low vegetation types such as shrubs and grasslands (Supplementary Figure C.2a, Appendix C.1). While GLEAM-HR shows similar values of approximately 500 mm·year⁻¹ in this region, its two spatial maxima occur eastwards, in the national parks of Heuvelrug (52.25°N–5.25°E) and the Veluwe (52.25°N–5.75°E), both densely-forested regions as can be seen in Supplementary Figure C.2a (Appendix C.1). The dense vegetation together with the high precipitation volumes in the region (ter Maat *et al.*, 2013) result in large fluxes of transpiration and rainfall interception loss. This effect is also apparent in smaller forested areas in the south and east of The Netherlands. Note that this pattern is not captured by LSA-SAF, as rainfall interception loss is not explicitly modelled, plus it occurs during cloudy periods when retrievals from Meteosat are either not available, or of lower quality.

4.4.3 Summer drought 2013

In 2013, only 740 mm of precipitation was recorded over The Netherlands, approximately 100 mm less than the long-term multi-annual average (<https://www.knmi.nl/>; last visit: 22 November 2019). The year 2013 can thus be considered as a relatively dry year, with below-average precipitation during January–April and June–August. As discussed in Section 4.4.2, soil-water availability is generally not affecting the evaporation rate in The Netherlands. Hence, potential evaporation is maintained for large parts of the year; i.e. the surface is able to supply the atmospheric demand for water (Jacobs *et al.*, 2010; Jacobs and De Bruin, 1998; De Bruin, 1981). However, during dry spells, soil water can be exceptionally low, resulting in evaporative water stress and a consequent reduction in terrestrial evaporation as compared to its potential rate. In addition, below-average rainfall also results in reductions of rainfall interception loss, which substantially affect the total evaporative flux in forested regions.

Figure 4.6a shows the anomaly of the cumulative evaporation curve for 2013 (averaged over The Netherlands), relative to the multi-annual (2013–2017) mean for GLEAM-HR, LSA-SAF, and the Makkink data set. The annual volume of evaporation in 2013 is approximately 20 mm (-4.5%, LSA-SAF), 25 mm (-4%, Makkink), and 28 mm (-5.5%, GLEAM-HR) less than the climatological mean of each product. While these volumes are relatively similar, each data set shows substantially different temporal dynamics in the anomaly time series, especially during summer (Figure 4.6a), when evaporation volumes are higher and the rainfall anomaly is stronger. The Makkink data set shows a decrease

in the curve at the beginning of summer, but an increase from July onward, following the dynamics of surface net radiation (Figure 4.7a). LSA-SAF shows a relatively horizontal curve during summer, indicating that – averaged over The Netherlands – evaporation is close to normal during this period. Finally, GLEAM-HR shows a decreasing trend in the curve during all summer months, with the steepest decrease in August–September, coinciding with the strongest anomaly in precipitation (Figure 4.7a).

Maps in Figure 4.6b reveal that the spatial response of terrestrial evaporation to the 2013 summer drought also differs substantially per product. As expected, the Makkink data set does not respond to the drought in 2013 and fully follows the radiation patterns (Figures 4.7b), resulting in below-average evaporation in June, and above-average evaporation in July and August. LSA-SAF and GLEAM-HR both consider a soil-water constraint on evaporation, and do respond to the rainfall deficits. However, the spatial patterns of the evaporation anomalies in both data sets are substantially different, with in general, a more conservative response of LSA-SAF (compared to GLEAM-HR) to the rainfall anomalies. Note that the patterns in LSA-SAF can generally not be related to the precipitation and radiation anomalies shown in Figure 4.7, suggesting that other variables used to force the algorithm are responsible for driving the patterns.

Evaporation anomalies from GLEAM-HR (Figure 4.6b) during the summer drought mainly follow the anomalies in the estimated soil moisture from GLEAM-HR (Supplementary Figure C.3, Appendix C.1), which are strongly affected by the rainfall patterns (Figure 4.7b). As shown, negative anomalies in evaporation as a result of water stress first develop in sandy soils (Supplementary Figure C.2b, Appendix C.1), characteristic of their low water-holding capacity. This effect can clearly be observed in August, when the cumulative rainfall deficit almost reaches its maximum (Figure 4.7a): while root-zone soil moisture anomalies are negative throughout the country, the strongest evaporation anomalies are found in sandy soils, while anomalies in clayey soils more towards the west are positive. The latter is explained by the larger water-holding capacity of these soils. Although the root-zone soil moisture is strongly depleted and anomalously low, soil water is still available to (partly) meet the atmospheric demand for water set by the positive anomaly in net radiation (Figure 4.7b).

The different response of LSA-SAF and GLEAM-HR to rainfall deficits can be explained by differences in the parameterisation of soil moisture stress. While GLEAM-HR adopts a relatively simple (non-linear) stress curve (Section 3.2.3), LSA-SAF uses the more complex – yet still empirical – Jarvis function to calculate stomatal conductance and to convert potential into actual evaporation (Ghilain *et al.*, 2011; Jarvis *et al.*, 1976). Also differences in forcing and forcing uncertainty affect the response of terrestrial evaporation to drought

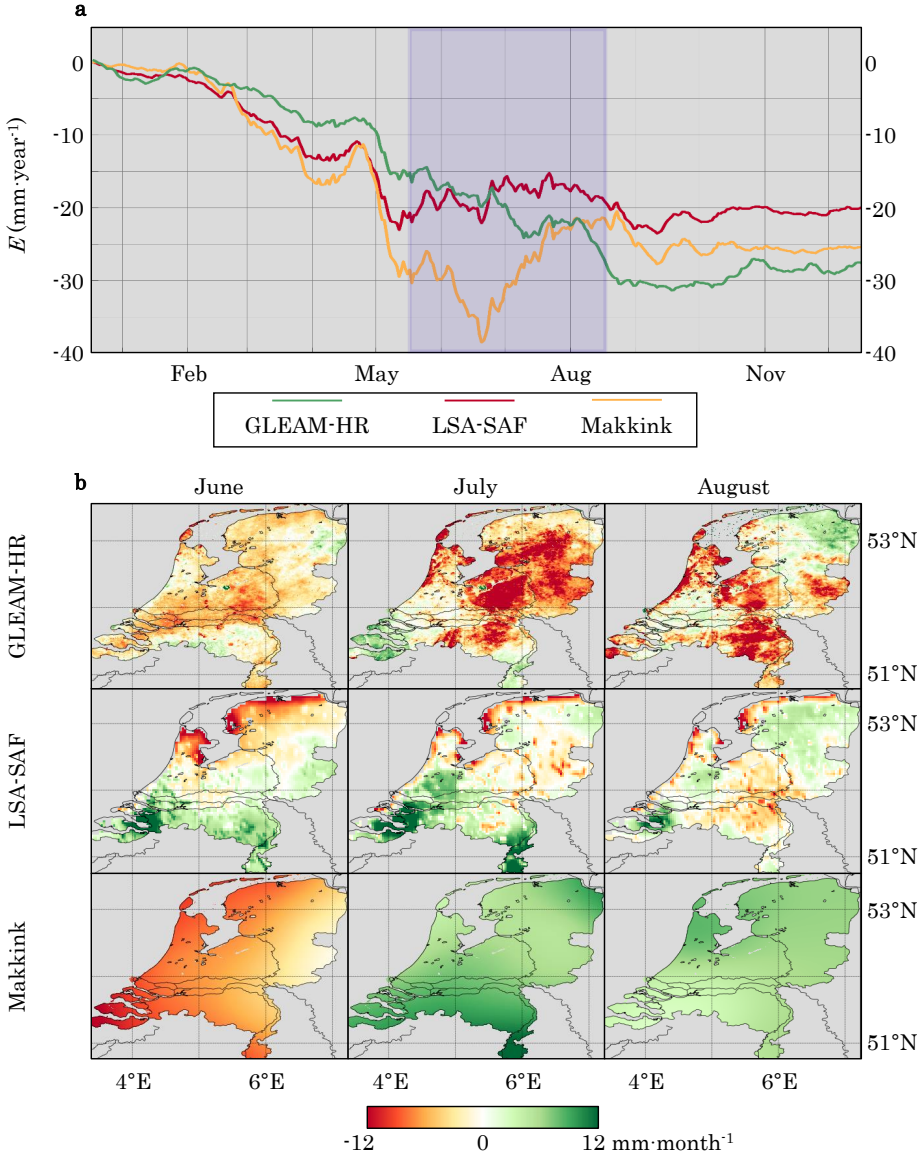


Figure 4.6: Anomalies of terrestrial evaporation in 2013. **(a)** Anomalies of the spatially-averaged, cumulative evaporation curve for 2013 (relative to the 2013–2017 yearly mean) for GLEAM-HR, LSA-SAF, and the Makkink data set. The shaded area corresponds to the months June–August. **(b)** Maps of the monthly anomalies (relative to the 2013–2017 monthly mean) of terrestrial evaporation from GLEAM-HR, LSA-SAF, and the Makkink data set for June–August 2013 in The Netherlands.

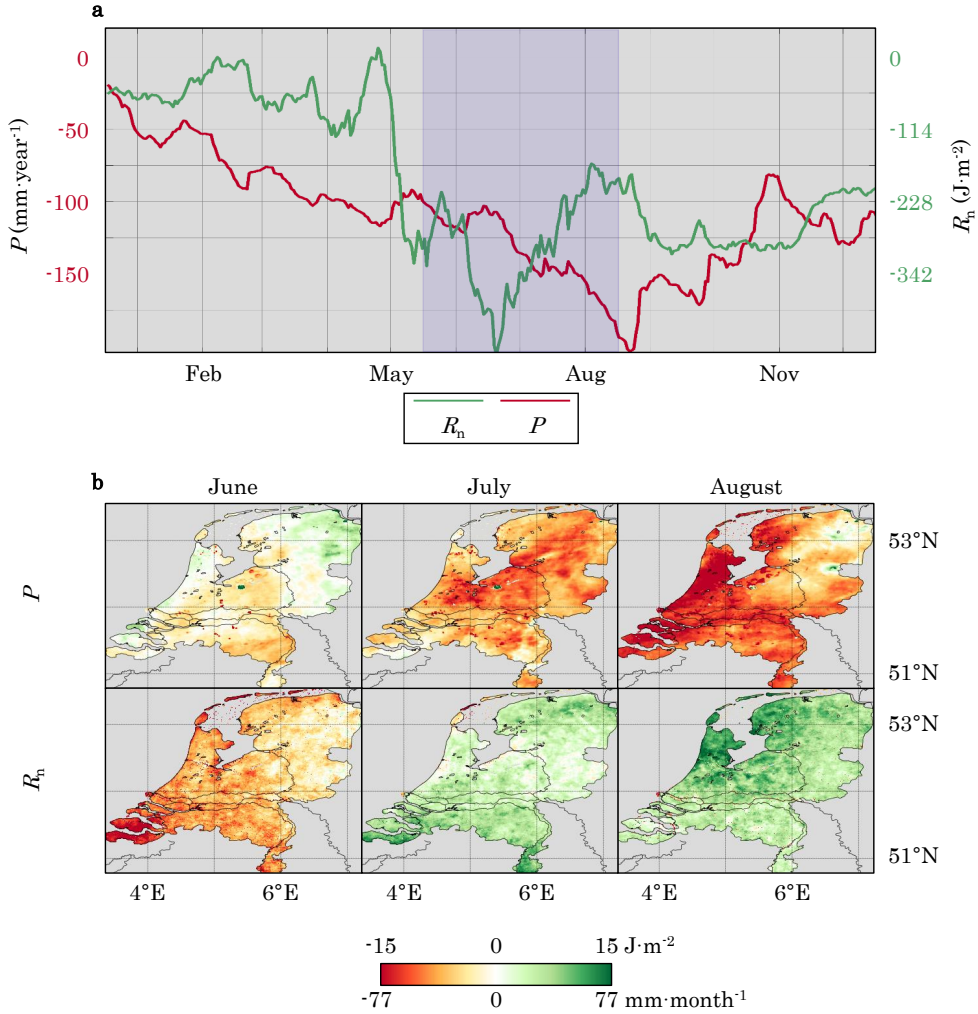


Figure 4.7: Anomalies of precipitation (P) and surface net radiation (R_n) in 2013. (a) Anomalies of the spatially-averaged, cumulative precipitation and net radiation curve for 2013 (relative to the 2013–2017 yearly mean). The shaded area corresponds to the months June–August. (b) Maps of the monthly anomalies (relative to the 2013–2017 monthly mean) of precipitation and surface net radiation for June–August 2013 in The Netherlands.

conditions. In GLEAM-HR, root-zone soil moisture is internally calculated using a simple water-balance model, forced by high-resolution observations of precipitation, and updated using a soil moisture data assimilation system. In contrast, in LSA-SAF, root-zone soil moisture is obtained from the ECMWF operational forecast model which provides data at substantially coarser spatial resolution than the target resolution of LSA-SAF (Ghilain *et al.*, 2011).

Given the high spatial variability of root-zone soil moisture as a result of the heterogeneity in soil properties, vegetation cover, and (to a lesser extent) atmospheric forcing, the coarse-scale soil moisture in LSA-SAF thus underestimates this variability and its impact on evaporation. Also note that in addition to the differences in soil moisture stress resulting in reduced transpiration and soil evaporation, GLEAM-HR also considers rainfall interception loss which strongly affects the total evaporation in densely-forested areas.

4.5 Conclusion

GLEAM is a relatively simple process-based model originally designed to estimate terrestrial evaporation for climatological studies, running at coarse resolution and global scales (Miralles *et al.*, 2011b). This study evaluated for the first time the potential of GLEAM to be applied at field scales. As such, the model was forced using all-weather, high-resolution inputs (100 m) over The Netherlands, Flanders, and the west of Germany, and the estimates of root-zone soil moisture and terrestrial evaporation from GLEAM-HR were evaluated against a sample of in situ measurements from soil moisture sensors (29 sites) and eddy-covariance towers (5 sites). In addition, GLEAM-HR was compared against the coarse-scale GLEAM v3.2b product (± 25 km), the LSA-SAF evaporation product (± 5 km), and the Makkink evaporation product from KNMI (10 km). Spatial patterns were also inter-compared, and their ability to respond to water stress was evaluated during the summer of 2013.

The temporal evaluation of GLEAM-HR against in situ data showed the ability of the model to retrieve temporal dynamics of surface soil moisture, as indicated by a median R and ubMAD across all sensors of 0.76 and $0.04 \text{ m}^3 \cdot \text{m}^{-3}$, respectively. In addition, the relatively simple data assimilation system in GLEAM-HR was able to extract valuable information from the microwave observations of soil moisture, yielding a mild improvement in the temporal dynamics. Meanwhile, the coarse-resolution GLEAM v3.2b showed equally realistic temporal dynamics in soil moisture, with even a slightly better performance than GLEAM-HR in regions outside the The Netherlands, where the quality of the ground-based radar rainfall product – used as an input in GLEAM-HR – is lower.

The estimates of terrestrial evaporation from GLEAM-HR were validated against measurements from five eddy-covariance sites, resulting in correlation coefficients ranging between 0.65 and 0.95, comparable to the statistics from GLEAM v3.2b, LSA-SAF, and the Makkink data set from KNMI. Estimates from GLEAM-HR appeared bounded by the low values from LSA-SAF and the high values from the Makkink data set. Despite the similar temporal validation statistics, an in-depth analysis of the spatial patterns in evaporation yielded remarkable differences across all four data sets. The Makkink product showed

almost no spatial variability due to its smoothing spline interpolation of a short range of in situ estimates, and GLEAM v3.2b showed only little spatial detail as a result of its coarse resolution. Both LSA-SAF and GLEAM-HR presented higher spatial heterogeneity, but patterns were different due to diverging model parameterisations, model assumptions, and forcing data. The most prevalent difference was attributed to the detailed modelling of rainfall interception loss in GLEAM-HR, an important flux in forested regions which is not well captured in LSA-SAF. As a result, the annual maximum evaporation from GLEAM-HR occurred in the national parks of the Veluwe and Heuvelrug, located in the center of The Netherlands, and both densely-forested regions. In contrast, LSA-SAF showed its maximum in the Green Heart of The Netherlands, a region dominated by lower vegetation types such as grasslands and shrubs.

Finally, the response of terrestrial evaporation to the 2013 summer drought in The Netherlands was also evaluated. While the Makkink product is only constrained by surface net radiation and does not respond to changes in precipitation, both LSA-SAF and GLEAM-HR showed below-average evaporative fluxes in the epicentre of the drought. However, the negative anomalies of GLEAM-HR were larger, presumably as a result of the higher sensitivity of terrestrial evaporation to root-zone soil moisture and differences in forcing data.

Overall, GLEAM-HR produced qualitative and spatially consistent estimates of root-zone soil moisture and terrestrial evaporation at spatial resolutions useful for agricultural and water management purposes. Because the algorithm is designed to rely (to a large extent) on microwave-based data sets of environmental forcing variables, resulting in all-weather output, it has an indisputable advantage over more traditional approaches applied at regional scales based on optical and TIR data. The reliance on a Priestley and Taylor framework makes it feasible to run on remote sensing observations only, and avoids the need for reanalysis data like other remote sensing models designed for the large-scale monitoring of evaporation.

Evaluating the surface energy partitioning in ERA5

In this chapter, the accuracy of surface energy partitioning in ERA5 is explored and compared to its predecessor ERA-I. To this end, the surface latent heat flux, surface sensible heat flux, and Bowen ratio are first validated against in situ eddy-covariance measurements. Furthermore, the same variables are evaluated against catchment-scale data derived using the water and energy-balance equation, together with measurements of river discharge. Finally, GLEAM is used as a tool to evaluate the skill of the land surface model in the reanalysis scheme. This chapter is an edited version of the following scientific publication in review:

Martens, B., Schumacher, D.L., Wouters, H., Muñoz-Sabater, J., Verhoest, N.E.C., Miralles, D.G., 2019. Evaluating the surface energy partitioning in ERA5. *Geoscientific Model Development Discussions*, *in review*.

5.1 Introduction

The partitioning of available energy at the land surface into sensible and latent heat translates variations in the state of the land surface (e.g. soil moisture) into changes in the state of the atmosphere (e.g. cloud formation, near-surface air temperature, and the atmospheric boundary layer height) at local, but also remote locations (Teuling *et al.*, 2017; Miralles *et al.*, 2016; Guillod *et al.*, 2015; Taylor *et al.*, 2012; Seneviratne *et al.*, 2010). Hence, surface energy partitioning is a crucial process in the occurrence and development of extreme events such as droughts and heatwaves (Miralles *et al.*, 2019, 2014; Teuling *et al.*, 2010; Seneviratne *et al.*, 2006). An accurate representation of the processes involved in this partitioning in land surface models is thus essential to advance our understanding of past variations in climate, and leverage our abilities to predict future climate and its impacts on our biosphere (Berg and Sheffield, 2018; Dirmeyer *et al.*, 2018).

Climate reanalyses are data sets describing the past and present state of our climate system and are derived using coupled numerical models in which a vast amount of observations is ingested through a state-of-the-art data assimilation system. Although largely constrained by observations, the data remains model-based and the quality varies through time, depending on the accuracy and number of observations assimilated into the system (Hersbach *et al.*, 2019; Dee *et al.*, 2011). Reanalyses typically cover multi-decadal periods and are produced using a model setup and data assimilation framework (often referred to as the Integrated Forecast System, IFS, at ECMWF) that is fixed in time, resulting in consistent data sets describing the recent state of the atmosphere, ocean, and land surface at the global scale. Therefore, reanalyses are widely used to study past climate, derive long-term records of essential climate variables, initialise climate or Earth system models, or force land surface models offline. The latter may result in higher-resolution specialised land surface reanalyses (Muñoz Sabater, 2019; Albergel *et al.*, 2018; Reichle *et al.*, 2017; Balsamo *et al.*, 2015). During the last decade, several climate reanalyses have been produced, such as NASA’s MERRA-2 (Gelaro *et al.*, 2017), the Japanese 55-year ReAnalysis (JRA-55; Kobayashi *et al.*, 2015) from the Japanese Meteorological Agency (JMA), and ECMWF’s ERA-I (Dee *et al.*, 2011). Recently, ECMWF released ERA5 (Hersbach *et al.*, 2019), a new global climate reanalysis currently spanning the period 1979–present, which serves as the successor of ERA-I¹. ERA5 is produced using an enhanced modelling and data assimilation framework and it benefits from the assimilation of a significantly higher number of observations compared to ERA-I. In addition, the archive will soon cover the period 1950–present and data will become available with a latency of 2 to 4 days. Finally, data are provided at a higher

¹Production of ERA-I was stopped in August 2019.

spatial (31 km vs. 80 km) and temporal (hourly vs. 3-hourly) resolution than ERA-I. Note that in case of ERA-I, the 3-hourly resolution can, in fact, only be obtained by combining forecast and analysis steps (Dee *et al.*, 2011).

The number of studies evaluating the quality of different variables from ERA5 is still limited. Yet, results generally point to improvements upon its predecessor and a better quality than other existing reanalyses for various surface and atmospheric variables. Tetzner and Thomas (2019), for instance, evaluated several meteorological variables from ERA5 and ERA-I, such as near-surface air temperature and wind speed, over the southern Antarctic peninsula, and concluded that the better spatio-temporal resolution at which physical processes are re-solved in ERA5 positively affects the representation of these variables. These results were confirmed by Wang *et al.* (2019), who compared the quality of a similar set of near-surface meteorological variables from ERA5 and ERA-I by means of in situ validation and a modelling exercise, where a thermodynamic sea-ice model was forced with reanalysis data over the Arctic ice sheet. Jiang *et al.* (2019) and Urraca *et al.* (2018) validated ERA5 radiation components against in situ measurements and compared their quality to other reanalyses, ground-based observations, and satellite data. Although a small positive bias still remains in ERA5 surface irradiance – mainly due to errors in the simulation of cloud properties – that bias is significantly lower than in ERA-I and MERRA-2, especially at inland locations (Urraca *et al.*, 2018). However, in more complex terrain such as mountainous or coastal regions, the authors concluded that high-resolution regional-scale reanalyses, such as the COnsortium for Small-scale MOdeling (COSMO) REAnalysis version 6 (COSMO-REA6) from the German weather service, perform better than ERA5. Also surface wind fields have been shown to be accurately represented in ERA5 (Olauson, 2018), mainly as a result of the relatively high spatial resolution. Other studies have focused on the validation of vertical profiles of atmospheric properties such as humidity and temperature, typically revealing that the representation of these fields is better in ERA5 than in various other data sets, including its predecessor ERA-I (e.g. Brunamonti *et al.*, 2019; Graham *et al.*, 2019; Zhang and Cai, 2019). Finally, Albergel *et al.* (2018) compared the quality of ERA-I and ERA5 by forcing the Interactions between Soil, Biosphere, and Atmosphere (ISBA) land surface model with meteorological fields derived from both reanalyses and comparing the simulated land surface variables from ISBA to independent data from satellite observations and in situ measurements. Based on their study, Albergel *et al.* (2018) concluded that forcing the model with ERA5 yielded consistently better estimates of hydrological states and fluxes.

Despite the importance of an accurate representation of the processes involved in the surface energy partitioning, at present, no study has directly evaluated the partitioning of energy in ERA5 into the two major surface

turbulent fluxes (i.e. the sensible and latent heat fluxes). As surface energy partitioning acts as a nexus between the land surface and atmosphere, such an analysis might provide useful insights to further improve the modelling of this coupled system, and to advance the quality of future reanalyses. Therefore, the objective of this chapter is to evaluate the ERA5 surface turbulent fluxes (and their ratio; i.e. the Bowen ratio) for the period 1983–2014 at the global scale. Several experiments are conducted using various independent observational data sets and using GLEAM as a modelling tool, to evaluate these variables from point to catchment-scale and sub-daily to yearly scales over the global land surface. The chapter is organised as follows: in Section 5.2, the experimental setup and the data sets used in the study are described, together with a brief overview of the key differences between ERA-I and ERA5. In Section 5.3, results of the experiments are discussed and the quality of surface energy partitioning in both reanalyses is assessed. Finally, concluding remarks are summarised in Section 5.4.

5.2 Methods and data

5.2.1 ERA5 and ERA-I data

ERA5 is the latest state-of-the-art reanalysis produced at ECMWF (Hersbach *et al.*, 2019), replacing the widely-used ERA-I (Dee *et al.*, 2011). A first segment of the data set, covering the period 2010–2016, was released early 2017, about a decade after the successful release of ERA-I. Compared to ERA-I, which uses IFS cycle 31r1, ERA5 is produced using an improved version of ECMWF’s modelling and data assimilation system (IFS cycle 41r2) and ingests information from a substantially larger volume of improved observations, resulting in a high-quality reanalysis of global atmospheric, oceanic, and land surface fields at hourly time steps, 137 vertical pressure levels, and horizontal resolution of approximately 31 km. Several advancements upon ERA-I are expected to affect the surface energy partitioning in ERA5 (Hersbach *et al.*, 2019), including (1) a better forcing of solar irradiance, greenhouse gases, and stratospheric sulphate aerosols, which affect the available energy at the surface, (2) a substantially higher spatial resolution, allowing for a more realistic representation of surface-atmosphere interactions in complex terrain such as mountainous or coastal regions, and (3) an improved land surface model, namely the Hydrology Tiled ECMWF Scheme for Surface Exchanges over Land (H-TESSSEL), which has a demonstrated high skill to simulate surface turbulent heat fluxes in offline experiments (Balsamo *et al.*, 2015; Albergel *et al.*, 2012; Balsamo *et al.*, 2008). Note that H-TESSSEL is a more advanced version of the TESSSEL model implemented in ERA-I, with the main differences being a better description of infiltration and surface run off, a new algorithm to model snow dynamics, and a revised formulation of bare soil evaporation.

Here, the surface sensible heat flux, surface latent heat flux, and Bowen ratio derived from both ERA5 and ERA-I are evaluated globally for the period 1983–2014 (i.e. the period for which reference data are available; Sections 5.2.2 and 5.2.3) using independent in situ data and GLEAM as a modelling tool. Next to the turbulent fluxes and the Bowen ratio, precipitation, 2-meter air temperature, and surface radiation components (from which the surface net radiation is calculated) are processed. These variables are used to disentangle the role of the improved atmospheric data versus the more evolved land surface model in ERA5.

5.2.2 FLUXNET 2015

In situ eddy-covariance data for the turbulent fluxes are obtained from the FLUXNET 2015 synthesis data set covering the period 1991–2014. The data set is processed as in Section 3.3.2, including (1) masking of rainy intervals at hourly time steps to remove unreliable measurements due to wet sensors, (2) removing gap-filled data records, and (3) aggregating to both 3-hourly and daily temporal resolutions. Note that for the temporal aggregation, 20% of the higher resolution data within the interval are allowed to be missing. Aiming at the calculation of robust validation statistics, only sites with at least 365 daily records (i.e. at least one full year of data) after masking are retained, resulting in a validation sample of 143 (corresponding to roughly 760 site years) quality-checked eddy-covariance sites. The location of these sites is shown in Figure 5.1 and a list is provided in Table A.4 (Appendix A). Note that the same set of towers is used in the sub-daily (i.e. 3-hourly) and daily evaluations of the turbulent fluxes, making the validation metrics between experiments inter-comparable. As the temporal variability of the turbulent fluxes is strongly influenced by the seasonal cycle of its main drivers, the performance of the land surface scheme in response to anomalous weather conditions (i.e. with respect to the seasonal cycle) might be masked when raw time series are analysed. As such, most of the analyses in this chapter are based on standardised anomalies to better evaluate the skill of ERA5 in capturing the effect of specific meteorological conditions on the surface energy partitioning. Note that standardised anomalies are preferred here over regular anomalies to make statistics of different variables – ranging in different order of magnitudes – comparable. To calculate the climatology, only FLUXNET sites with a minimum record length of five years are considered, resulting in 77 eddy-covariance towers when anomalies are used for validation (Figure 5.1). Note that about 50% of these selected sites have a record length of more than 10 years, with a maximum of 21 years.

The Bowen ratio at each eddy-covariance site is calculated at daily temporal resolution as the ratio of the surface sensible heat flux and the surface latent heat flux. The Bowen ratio might be highly unstable when the turbulent

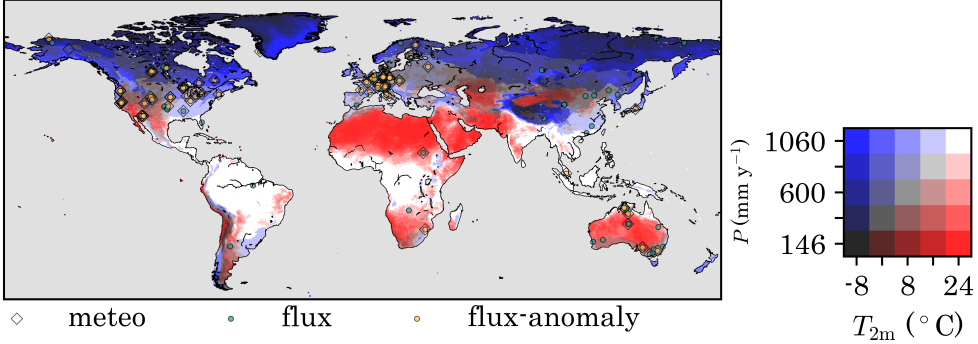


Figure 5.1: Location of the selected eddy-covariance sites. Sites with a record length of less than 5 years (i.e. where no anomalies are calculated) are plotted in green and sites with a record length of more than 5 years (i.e. where anomalies are calculated) are plotted in yellow. Sites where measurements of meteorological data are also available are indicated with a diamond. The background provides information on the climatological mean temperature and precipitation derived from ERA5 (1983–2018).

fluxes are small compared to the measurement error of the eddy-covariance system, even at the daily temporal resolution. Therefore, outliers in the in situ time series of the Bowen ratio are masked by removing records outside the following window: $[q_{25} - 1.5(q_{75} - q_{25}); q_{75} + 1.5(q_{75} - q_{25})]$, where q_{75} and q_{25} are the 75% and 25% quantiles of the Bowen ratio time series, respectively (the same procedure is used in e.g. Section 2.3.1). Next to the turbulent fluxes, measurements of surface net radiation, near-surface air temperature, and precipitation at the eddy-covariance sites are processed the same way, except for the masking of rainy intervals. These variables are typically not recorded at each eddy-covariance site and are therefore only available at 83 sites in total (Figure 5.1).

For each eddy-covariance site in the validation data set, the variables from the corresponding ERA5 and ERA-I grid cell are extracted at their original spatial resolution and both as 3-hourly and daily (temporal) aggregates. The Bowen ratio from both reanalyses is calculated and processed in a similar manner as for the in situ data; i.e. only at the daily temporal scale and outliers are removed. Eddy-covariance sites located within the same grid cell of the reanalysis are treated separately in the validation to avoid potential problems resulting from merging sensors with different absolute values and gaps in their record, similar as in Section 3.3.2. The quality of the surface energy partitioning in both reanalyses is then assessed by calculating the MD, MAD, and Pearson correlation coefficient against the in situ data for the period 1991–2014.

5.2.3 Catchment water and energy-balance data

If changes in water storage are neglected, the catchment-scale evaporative flux can be calculated as precipitation minus river discharge (Equation 1.1); both averaged over a sufficiently long time period (Miralles *et al.*, 2016; Liu *et al.*, 2014; Wang and Dickinson, 2012; Miralles *et al.*, 2011b; Vinukollu *et al.*, 2011). By taking into account the latent heat of vaporisation and the density of water:

$$\lambda\rho E = \lambda\rho(P - Q) \quad (5.1)$$

The assumption that changes in catchment water storage can be ignored requires the consideration of a sufficiently long period compared to the concentration time of the catchment; as in Miralles *et al.* (2016), a yearly aggregation period will be considered here.

A similar reasoning as for the catchment mass balance can be made in terms of energy balance: when changes in energy storage can be neglected, the energy balance at the catchment implies that the surface sensible heat flux can be calculated as the difference between surface net radiation and the sum of ground and latent heat fluxes (Equation 1.2):

$$H = R_n - (G + \lambda\rho E) \quad (5.2)$$

Combining Equations 5.1 and 5.2 thus provides a means to evaluate the long-term average catchment-scale Bowen ratio, derived from surface net radiation, ground heat flux, precipitation, and river discharge as:

$$\beta_b = \frac{(R_n - G)}{\lambda\rho(P - Q)} - 1, \quad (5.3)$$

where β_b (–) is the Bowen ratio.

In this chapter, Equations 5.1–5.3 are used in combination with an observational data set of river discharge covering the period 1983–2014 to derive an annual benchmarking data set of the turbulent fluxes and Bowen ratio at the catchment scale. Discharge measurements are obtained from the Global Runoff Data Centre (GRDC), providing data for nearly 4000 catchments with a daily or monthly temporal resolution. As in Miralles *et al.* (2016), records with data artifacts are first removed based on an exhaustive visual screening, and only catchments with an area larger than 2500 km² are considered. In addition, only catchments with a gridded area (on a regular 0.25° latitude–longitude grid) deviating less than 20% from the area reported by GRDC are retained. If measurements are recorded at multiple locations and thus for different drainage areas (particularly in Central Europe), measurements further downstream are favoured. By doing so, catchments are selected without any spatial overlap (due to possible sub-catchments measured upstream). After this initial filtering, data available at the daily scale are first aggregated to monthly values, given

that at least 25 days per month are present. To reduce the impact of e.g. human disturbances such as large-scale groundwater pumping or regulations of river flow, non-overlapping moving windows containing monthly data of 15 years are calculated. Any catchment for which the average of a window is exceeded more than three standard deviations by the mean of the subsequent window are discarded, to remove catchments where obvious disturbances occur during the study period. Finally, monthly averages are aggregated to annual averages, conditioning on at least 10 months per year being present.

Surface net radiation and precipitation to derive catchment-scale validation data for the turbulent fluxes and the Bowen ratio using Equations 5.1–5.3 are taken from the respective reanalysis in order to evaluate the effect of the land surface scheme in the IFS on the surface energy partitioning, rather than the combined effect of the atmospheric and land surface model. The ground heat flux is calculated as a fixed fraction of the surface net radiation depending on the land cover as in Martens *et al.* (2017, 2016), using the Global Vegetation Continuous Fields product (MOD44B v6; Dimiceli *et al.*, 2015a) derived from measurements of MODIS, and the open water product from Tuanmu and Jetz (2014).

For each catchment in the validation data set, the corresponding variables from ERA5 and ERA-I are extracted for the period 1983–2014. These data are spatially aggregated to the scale of the catchment and annual averages are calculated to match the temporal resolution of the validation data. Given the relatively low number of samples due to the annual temporal resolution (i.e. maximally 32 samples are available per catchment), only the bias in the reanalyses is assessed here by means of the percentage MD (%MD, i.e. MD divided by the mean of the reference data set). The latter validation metric is preferred over the MD as it allows to compare the bias between variables ranging in a different order of magnitude.

5.2.4 GLEAM

GLEAM is described in detail in Chapters 2 and 3. In this chapter, GLEAM v3 is used as a tool to assess quality differences in some key meteorological drivers of the turbulent fluxes, derived from ERA5 and ERA-I, and to explore the skill of the land surface model implemented in ERA5 (H-TESSEL) to accurately model the control of the land surface on the turbulent heat fluxes. To do so, GLEAM is forced with an updated version of the GLEAM v3.0a forcing data base described in Section 3.3.1, which uses near-surface air temperature and surface net radiation from ERA-I (hereafter referred to as GLEAM+ERA-I). Next, GLEAM is also forced using the same data set, but with near-surface air temperature and surface net radiation from ERA5 (hereafter referred to as GLEAM+ERA5). Although GLEAM has been designed to target the accurate estimation of terrestrial evaporation (or surface latent heat flux), here, the

surface sensible heat flux, calculated as the residual of the energy balance ignoring changes in energy storage (Equation 5.2), and the Bowen ratio from GLEAM are also evaluated. GLEAM is run for the period 1989–2015 at 0.25° spatial resolution and is initialised as described in Section 3.4, where 1989 is used as a spin-up year. The surface latent heat flux from both experiments (i.e. GLEAM forced with both reanalyses) is evaluated against the eddy-covariance data (Section 5.2.2) at the daily temporal scale. Note that the same validation statistics as described in Section 5.2.2 are calculated.

5.3 Results and discussion

5.3.1 Evaluation using eddy-covariance data

Direct comparison to in situ data

Figure 5.2 shows violin plots of the MD (raw in situ time series as reference), MAD_{san} (standardised anomaly in situ time series as reference), and R_{san} (standardised anomaly in situ time series as reference) of the turbulent fluxes and the Bowen ratio against in situ eddy-covariance measurements. Violin plots are presented for the surface latent heat flux (3-hourly and daily resolution), surface sensible heat flux (3-hourly and daily resolution), and Bowen ratio (daily resolution), for ERA5 (green) and ERA-I (yellow), respectively. As shown, statistics are consistently better for ERA5 than for ERA-I, with typically higher R_{san} and lower MAD_{san} against in situ measurements, even though the bias remains relatively similar. This indicates that ERA5 is better capturing the temporal dynamics in surface energy partitioning, both at sub-daily and daily temporal resolutions. Especially for the daily-aggregated surface sensible heat flux, a clear improvement can be seen, with the median R_{san} of ERA5 across all reference sites approaching the 75% percentile of the ERA-I distribution. For the surface latent heat flux and Bowen ratio, improvements are less remarkable, but still consistent. Notably, for both ERA-I and ERA5, validation statistics are generally better for sensible than for latent heat fluxes (see higher median R_{san} and lower MAD_{san} for sensible heat fluxes, irrespective of data set and temporal aggregation). Albeit the differences in pre-processing techniques and in the sample of eddy-covariance sites, these results are consistent with those by Balsamo *et al.* (2015) based on a validation of ERA-I only. When the seasonality is not removed (Supplementary Figure C.4, Appendix C.2), turbulent fluxes of ERA5 still outperform those from ERA-I, although differences are smaller. In terms of seasonal cycle, the surface sensible heat flux is not necessarily better estimated than the surface latent heat flux; in fact, statistics are generally worse at daily temporal resolution as shown in Supplementary Figure C.4 (Appendix C.2).

Figure 5.3 shows the difference between the temporal validation statistics

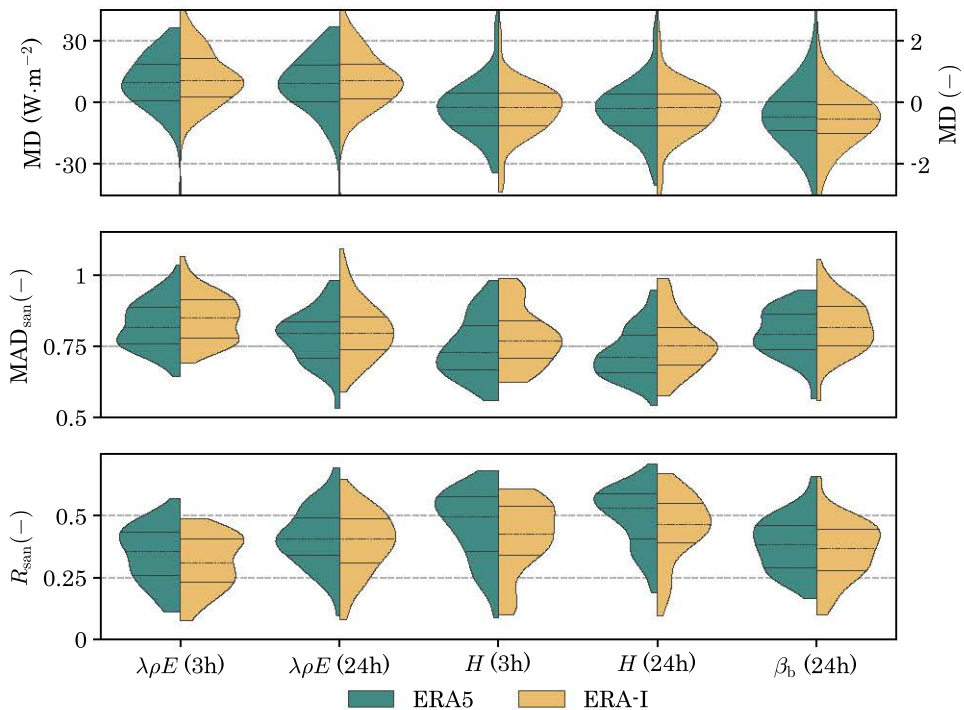


Figure 5.2: Violin plots of temporal validation statistics of the surface latent heat flux ($\lambda\rho E$), surface sensible heat flux (H), and Bowen ratio (β_b) from ERA5 (green) and ERA-I (yellow). Statistics are calculated against in situ eddy-covariance measurements at both 3-hourly and daily temporal resolutions. Violin plots represent the distribution of the individual validation statistics with indication of the median and inter-quartile range, and are calculated using a kernel density estimation approach. Statistics include the Mean Difference (MD, raw in situ time series from 143 sites as reference), Mean Absolute Difference (MAD_{san} , standardised anomaly in situ time series from 77 sites as reference), and the Pearson correlation coefficient (R_{san} , standardised anomaly in situ time series from 77 sites as reference). For MD, the distribution of β_b is plotted on the right y-axis.

(i.e. MAD_{san} and R_{san}) of the surface latent heat flux, surface sensible heat flux, and Bowen ratio from ERA5 and ERA-I. Sites are grouped as a function of mean annual precipitation and near-surface air temperature measured at the corresponding eddy-covariance site. Results are consistent with those in Figure 5.2, with an overall higher quality (green color) in the sensible and latent heat fluxes from ERA5. However, it can be argued that there is a tendency of ERA-I to perform better than ERA5 in warm and dry regimes, especially for the latent heat flux and Bowen ratio. These climates are, nonetheless, only sampled by three eddy-covariance towers and thus results may not be generalised. In addition, conclusions based on the performance in certain

climate regimes should be interpreted with care, as FLUXNET sites are not uniformly distributed: mild climates are generally over-represented and most sites are located in Europe and the CONUS, as shown in Figure 5.1 and described in Baldocchi *et al.* (2001).

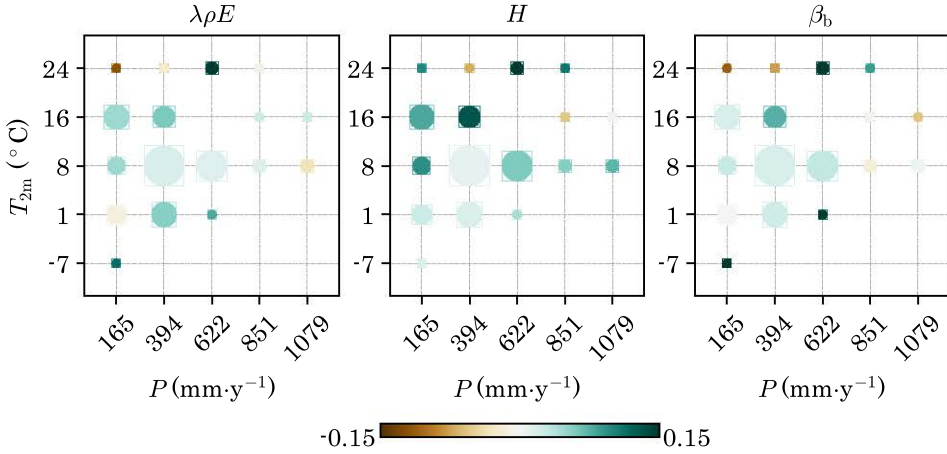


Figure 5.3: Difference between the temporal validation statistics of the surface latent heat flux ($\lambda\rho E$), surface sensible heat flux (H), and Bowen ratio (β_b) from ERA5 and ERA-I grouped as a function of precipitation rate (P) and near-surface air temperature (T_{2m}) calculated at the in situ site. Statistics are calculated against in situ eddy-covariance measurements at daily resolution and then averaged across the sites within each group. Statistics include the Mean Absolute Difference (MAD_{san} , standardised anomaly in situ time series from 77 sites as reference) and the Pearson correlation coefficient (R_{san} , standardised anomaly in situ time series from 77 sites as reference). Circles show the R_{san} from ERA5 minus the one from ERA-I, while squares show the MAD_{san} from ERA-I minus the one from ERA5; hence, green colors represent better statistics for ERA5 compared to ERA-I. The size of the symbols relates to the number of in situ sites per group.

Presumably, much of the improvement in surface energy partitioning in ERA5 over ERA-I can be attributed to the more advanced land surface model used in ERA5, H-TESEL. The better performance of H-TESEL – in reference to TESSEL, its antecessor used in ERA-I – was already illustrated by Balsamo *et al.* (2015), who compared the quality of different land surface variables, such as soil moisture and the turbulent fluxes, from ERA-I and ERA-I/Land over the Northern Hemisphere. ERA-I/Land is in essence an offline simulation of H-TESEL forced with atmospheric data derived from ERA-I. Although quality differences between ERA-I and ERA-I/Land cannot only be attributed to the land surface scheme but also to the different model setup (i.e. online vs. offline simulation), Balsamo *et al.* (2015) argued that most of the improvement was due to the land surface model. As H-TESEL is now also implemented in

ERA5, analogous improvements can thus be expected in ERA5 over ERA-I regarding the simulation of land surface variables.

Despite the fact that these studies have shown the high performance of H-TESSEL as compared to TESSEL for simulating different land surface variables (e.g. Balsamo *et al.*, 2015; Albergel *et al.*, 2012), Balsamo *et al.* (2015) also showed that in case of the turbulent fluxes, improvements of ERA-I/Land over ERA-I could not be uniquely linked to the improved land surface scheme. Hence, the better quality of surface energy partitioning in ERA5 is, most likely, not only owed to an improved parameterisation of the land surface, but also to a better quality of the atmospheric drivers, simulated by the coupled atmospheric model, which is constrained by a 4D-variational data assimilation of a large number of quality-controlled observations (Hersbach *et al.*, 2019). The better quality of some key meteorological variables is confirmed by the results presented in Supplementary Figure C.5 (Appendix C.2), which shows violin plots of the validation statistics for surface net radiation, 2-meter air temperature, and precipitation at the FLUXNET sites, for 3-hourly and daily temporal resolutions, respectively. Although statistics from ERA5 are better at both temporal resolutions, especially the sub-daily variability of all three variables has been substantially improved over ERA-I, which may largely be the result of a better modelling of cloud properties in ERA5 (Hersbach *et al.*, 2019).

Finally, as described in Section 5.2.1, one of the key improvements in ERA5 upon its predecessor is the higher spatial resolution at which atmospheric and land processes are resolved. However, Supplementary Figure C.6 (Appendix C.2) shows that when ERA5 is linearly re-sampled to the spatial resolution of ERA-I, statistics calculated against eddy-covariance measurements only change marginally. Nevertheless, such an analysis might not be representative of the added value of higher spatial resolutions as (1) a simple re-sampling of the model output does not properly represent the effect of the high-resolution numerical modelling, (2) the advantage of the better spatial resolution is expected to be the highest in complex terrain such as mountainous regions, coastal areas, or highly-heterogeneous landscapes, which are under-represented in the FLUXNET data base, and (3) representative errors – resulting from the relatively small footprint of eddy-covariance towers as compared to model grid cells – remain considerable at the spatial resolution of ERA5.

Evaluation using GLEAM

Forcing GLEAM with meteorological data derived from ERA5 and ERA-I provides a convenient and alternative means to evaluate and compare the quality of the reanalyses. Moreover, it facilitates an evaluation of the suitability of ERA5 to drive offline models explicitly designed to estimate land surface fluxes

(such as terrestrial evaporation in case of GLEAM). Figure 5.4a shows violin plots of the MD (raw in situ time series as reference), MAD_{san} (standardised anomaly in situ time series as reference), and R_{san} (standardised anomaly in situ time series as reference) of the turbulent fluxes and the Bowen ratio derived from GLEAM against in situ eddy-covariance measurements. Violin plots are shown for both turbulent fluxes and the Bowen ratio at daily temporal resolution; the violin limbs correspond to GLEAM forced with ERA5 (green) and ERA-I (yellow), respectively. Results presented in Figure 5.4a show that the estimates of the surface latent heat flux from GLEAM+ERA5 are consistently better than those from GLEAM+ERA-I, especially in terms of R_{san} and MAD_{san} , while the bias in both is comparable and close to zero on average. These findings support the ones discussed in Section 5.3.1, where it was found that some key meteorological drivers of the surface turbulent fluxes are in fact better represented in ERA5 than in ERA-I. In contrast, with the exception of the bias, statistics for the surface sensible heat flux and Bowen ratio are slightly worse for GLEAM+ERA5 than for GLEAM+ERA-I. Nonetheless, when the seasonal cycle is not removed prior to the analysis (Supplementary Figure C.7a, Appendix C.2) GLEAM+ERA5 performs consistently (albeit only slightly) better for all variables, suggesting that the seasonality of the meteorological variables used to force GLEAM is better captured in ERA5 than in ERA-I. Despite the fact that the most prominent differences in quality of the surface latent heat flux from GLEAM+ERA5 and GLEAM+ERA-I can be found in mild climates as indicated in Figure 5.5a, there is no clear tendency of GLEAM+ERA5 to perform better under specific climatic conditions. Contrary, the surface sensible heat flux and Bowen ratio from GLEAM+ERA5 tend to degrade in quality (compared to GLEAM+ERA-I) when the climate gets drier and colder. It should be emphasised here again that GLEAM has been specifically designed to estimate the latent heat flux, thus the surface sensible heat flux – calculated here as the residual from the energy balance – has not been subject to equally extensive validations than its latent counterpart, and is prone to be more uncertain.

The turbulent fluxes and Bowen ratio from GLEAM+ERA5 can also be directly compared to ERA5 to provide a rough evaluation of the skill of H-TESEL as compared to the simpler land surface scheme in GLEAM. Figure 5.4b shows that ERA5 is better capturing the temporal dynamics of the anomalies, generally resulting in lower MAD_{san} and higher R_{san} for all variables. Only in terms of the bias, ERA5 is overall performing worse than GLEAM+ERA5, especially for the surface latent heat flux, which is consistently overestimated in ERA5 for almost all in situ sites (close to 75% of the sites have a positive bias, Figure 5.4b). This results in a median MD of $9 \text{ W}\cdot\text{m}^{-2}$ compared to the slight underestimation of $-2 \text{ W}\cdot\text{m}^{-2}$ for GLEAM+ERA5 at daily time scales. The positive bias in the surface latent heat flux from ERA5 is very

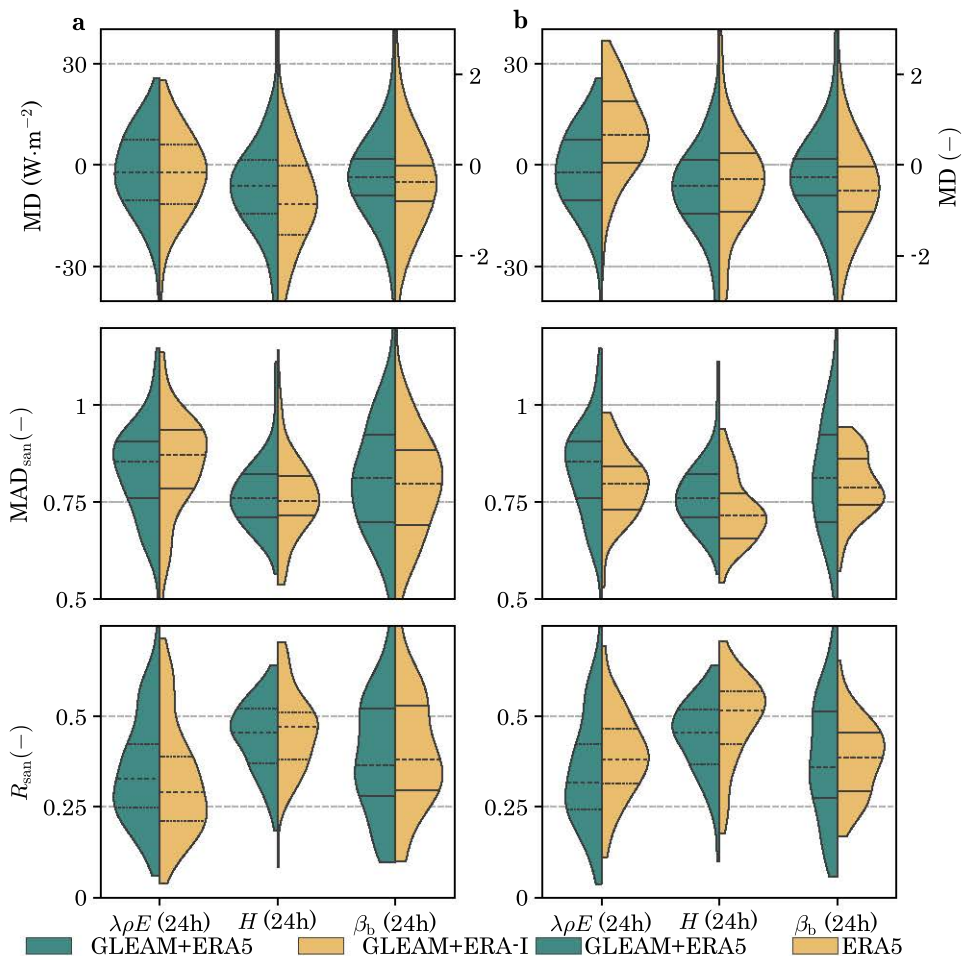


Figure 5.4: Violin plots of temporal validation statistics of the surface latent heat flux ($\lambda\rho E$), surface sensible heat flux (H), and Bowen ratio (β_b) from GLEAM+ERA5, GLEAM+ERA-I, and ERA5. **(a)** Compares the violin plots from GLEAM+ERA5 and GLEAM+ERA-I and **(b)** compares the violin plots from GLEAM+ERA5 and ERA5. Statistics are calculated against in situ eddy-covariance measurements at daily temporal resolution. Violin plots represent the distribution of the individual validation statistics with indication of the median and inter-quartile range, and are calculated using a kernel density estimation approach. Statistics include the Mean Difference (MD, raw in situ time series from 143 sites as reference), Mean Absolute Difference (MAD_{san}, standardised anomaly in situ time series from 77 sites as reference), and the Pearson correlation coefficient (R_{san} , standardised anomaly in situ time series from 77 sites as reference). For MD, the distribution of β_b is plotted on the right y-axis.

similar to the one from ERA-I, with a median MD of $10 \text{ W}\cdot\text{m}^{-2}$ across all

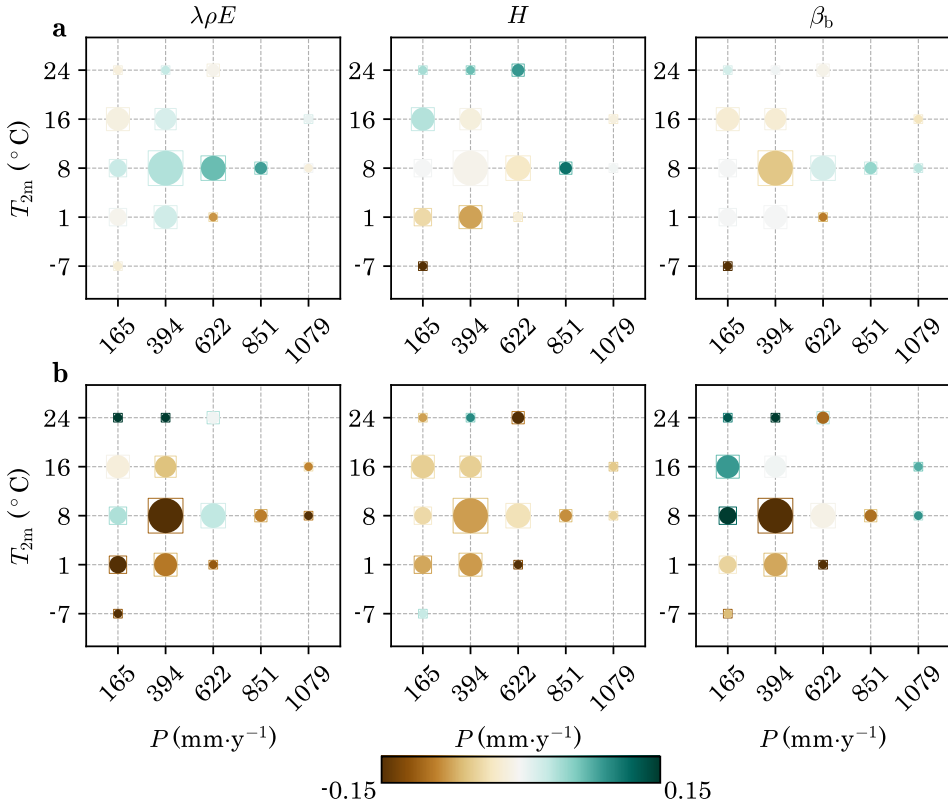


Figure 5.5: Difference between the temporal validation statistics of the surface latent heat flux ($\lambda\rho E$), surface sensible heat flux (H), and Bowen ratio (β_b) from GLEAM+ERA5, GLEAM+ERA-I, and ERA5 grouped as a function of precipitation rate (P) and near-surface air temperature (T_{2m}) calculated at the in situ site. **(a)** Compares the statistics from GLEAM+ERA5 and GLEAM+ERA-I and **(b)** compares the statistics from GLEAM+ERA5 and ERA5. Statistics are calculated against in situ eddy-covariance measurements at daily resolution and then averaged across the sites within each group. Statistics include the Mean Absolute Difference (MAD_{san} , standardised anomaly in situ time series from 77 sites as reference) and the Pearson correlation coefficient (R_{san} , standardised anomaly in situ time series from 77 sites as reference). In **(a)** circles show the R_{san} from GLEAM+ERA5 minus the one from GLEAM+ERA-I, while squares show the MAD_{san} from GLEAM+ERA-I minus the one from GLEAM+ERA5; hence, green colors represent better statistics for GLEAM+ERA5 compared to GLEAM+ERA-I. In **(b)**, statistics from GLEAM+ERA-I are replaced by ERA5; hence, green colors represent better statistics for GLEAM+ERA5 compared to ERA5. The size of the symbols relates to the number of in situ sites per group.

in situ sites at daily resolutions (Figure 5.2). The tendency to overestimate the latent heat flux in ERA-I has been previously reported in different stud-

ies (Michel *et al.*, 2016; Miralles *et al.*, 2016; Balsamo *et al.*, 2015; Decker *et al.*, 2012), and changes in the IFS have thus not been able to mitigate this bias in ERA5. Given the interaction between the coupled atmospheric and land surface model in the reanalysis, the consistent positive bias in the surface latent heat flux is potentially affected by both components of the modelling framework. Although it is hard to identify the exact cause of this bias, it might be induced by the overestimation of the number of wet days typically found in reanalysis data sets (Beck *et al.*, 2019), combined with precipitation rates that are often underestimated (Beck *et al.*, 2019), and vegetation density that might be overestimated (Král, 2011). This presumably results in an overestimation of the interception loss (Král, 2011), an important component of the total latent heat flux in densely-vegetated regions (Martens *et al.*, 2017; Miralles *et al.*, 2010). Note that this hypothesis is partially supported by our analysis: despite the fact that a positive bias can be found virtually everywhere, the strongest biases are typically found in densely-vegetated sites (not shown). We should emphasize here, however, that biases calculated against eddy-covariance measurements have to be interpreted with care, given the representativeness errors, and provided that turbulent heat fluxes are thought to be generally underestimated by the eddy-covariance technique, especially in case of the surface latent heat flux (Section 1.1.3). When the seasonal cycle is not removed prior to the evaluation (Supplementary Figure C.7b, Appendix C.2), GLEAM+ERA5 seems to perform equally good or slightly better than ERA5, indicating that GLEAM+ERA5 is marginally better than ERA5 at capturing the seasonal dynamics (Supplementary Figure C.7b, Appendix C.2), but worse at capturing the response of surface energy partitioning to short-term anomalies in meteorological conditions (Figure 5.4b).

Nonetheless, Figure 5.5b shows that for the surface latent heat flux, the better performance of ERA5 over GLEAM+ERA5 is mainly due to its better statistics in relatively wet or cold climatic regimes. In drier regimes and, especially warm regions (mainly located along the west coast of the CONUS and few eddy-covariance sites in Australia; Figure 5.1), GLEAM+ERA5 seems to better capture the anomalies of the surface latent heat flux, which might indicate that H-TESSSEL has room to improve the response to water stress. For the Bowen ratio, similar conclusions may be drawn, even though the quality of the sensible heat flux in ERA5 is consistently better than in GLEAM+ERA5.

5.3.2 Evaluation using catchment energy-balance data

As described in Section 5.2.3, observations of river discharge may be combined with precipitation, net radiation, and ground heat flux to derive catchment-scale and long-term estimates of the surface turbulent fluxes and the Bowen ratio, providing an alternative means to evaluate the surface energy partitioning in ERA-I and ERA5. Figure 5.6 compares the %MD of the surface latent heat

flux, surface sensible heat flux, and Bowen ratio (observations of catchment-scale variables as reference) from ERA5 and ERA-I using a scatter plot. The results shown in Figure 5.6 largely correspond to the ones shown in Figure 5.2 for the MD and point again to a substantial overestimation of the surface latent heat flux from ERA-I; in 83% of the catchments, a positive bias is obtained. Conversely, the surface sensible heat flux is generally underestimated (a negative bias is found in 61% of the catchments), resulting in an average underestimation of the catchment-scale Bowen ratio as well (a negative bias is found in 80% of the catchments). While absolute biases for the surface latent heat flux from ERA5 are lower than from ERA-I (an improvement is found in 75% of the catchments), ERA5 still overestimates the flux in most catchments. More striking are the results for the surface sensible heat flux: while ERA-I generally underestimates the flux, ERA5 overestimates it in about 70% of the catchments. In addition, the absolute bias of the surface sensible heat flux from ERA5 is higher than in ERA-I in 55% of the catchments. However, this potential overestimation is not confirmed by the in situ validation presented in Section 5.3.1 (Figure 5.2), where the surface sensible heat flux from both reanalyses appeared nearly unbiased. Finally, for the Bowen ratio, estimates of ERA5 appear better in about 60% of the catchments, arguably reflecting the improvement in the surface latent heat flux.

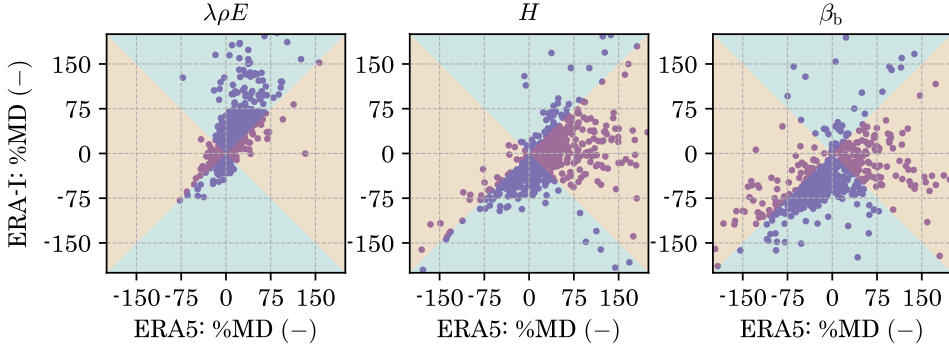


Figure 5.6: Scatter plot of the bias of the surface latent heat flux ($\lambda\rho E$), surface sensible heat flux (H), and Bowen ratio (β_b) from ERA-I versus ERA5. The bias is calculated against catchment-scale estimates of the fluxes derived using discharge data (Eqs. 5.1–5.3) and is assessed by the percentage Mean Difference (%MD, raw time series from 707 catchments as reference). The green area indicates catchments in which the bias in ERA5 is better than in ERA-I, and vice versa for the brown area.

Figures 5.7–5.9 show maps of the catchment-scale %MD of the surface latent heat flux (Figure 5.7), surface sensible heat flux (Figure 5.8), and Bowen ratio (Figure 5.9) for ERA5, ERA-I, and the difference in their absolute values. While ERA-I overestimates the surface latent heat flux virtually everywhere,

biases are largest in the east of the CONUS and the south of Europe (in regions like Spain and the south of France). In these regions, a strong reduction in bias can be observed for ERA5. Over large parts of Europe and western Russia, the surface latent heat flux from ERA5 is nearly unbiased, while the overestimation in other regions still remains, albeit reduced compared to ERA-I. Except for a small number of catchments in the northeast of Brazil and the west of the Sahel, the bias of the surface latent heat flux is lower in ERA5 than in ERA-I. The surface sensible heat flux from ERA-I is typically underestimated in high latitudes and the eastern part of the CONUS, while an overestimation can be seen in most other regions. However, as discussed in the previous paragraph, the bias in the surface sensible heat flux of ERA5 is typically higher, especially over Europe, western Russia, and the east of the CONUS; regions where the bias in the surface latent heat flux is reduced in ERA5.

Finally, it should be emphasised here that the quality of the catchment-scale sensible heat flux (and Bowen ratio) estimates used as reference (Section 5.2.3) is potentially lower than that of the surface latent heat flux, as (1) the assumption that the ground heat flux is a fixed fraction of the surface net radiation only affects the estimates of the sensible heat (Equation 5.2), and (2) the estimates of sensible heat flux depend on the estimates of surface latent heat (Equation 5.2), resulting in a propagation of errors which is difficult to assess. Hence, the catchment-scale evaluation of the surface sensible heat flux and Bowen ratio should be more carefully interpreted.

5.3.3 Global patterns of surface energy partitioning

Figure 5.10 shows maps of the multi-annual average of the surface latent heat flux, surface sensible heat flux, and Bowen ratio from ERA5 and ERA-I, as well as the difference between both. In both data sets, the expected geographical patterns set by the general climatic conditions emerge. High values for the surface latent heat flux can be found around the equator where both the availability of water and the supply of energy are high, while the lowest values can be found in arid regions such as the Sahara desert, central Australia, the Namibian desert, and the Gobi desert. In terms of surface sensible heat flux, an opposite pattern is shown, with relatively lower values in the tropics, where most of the available energy is consumed to evaporate water, and high values in the deserts, where virtually no water is evaporated. The Bowen ratio clearly marks the tropical forests and deserts; with intermediate values for mild climates such as central and western Europe.

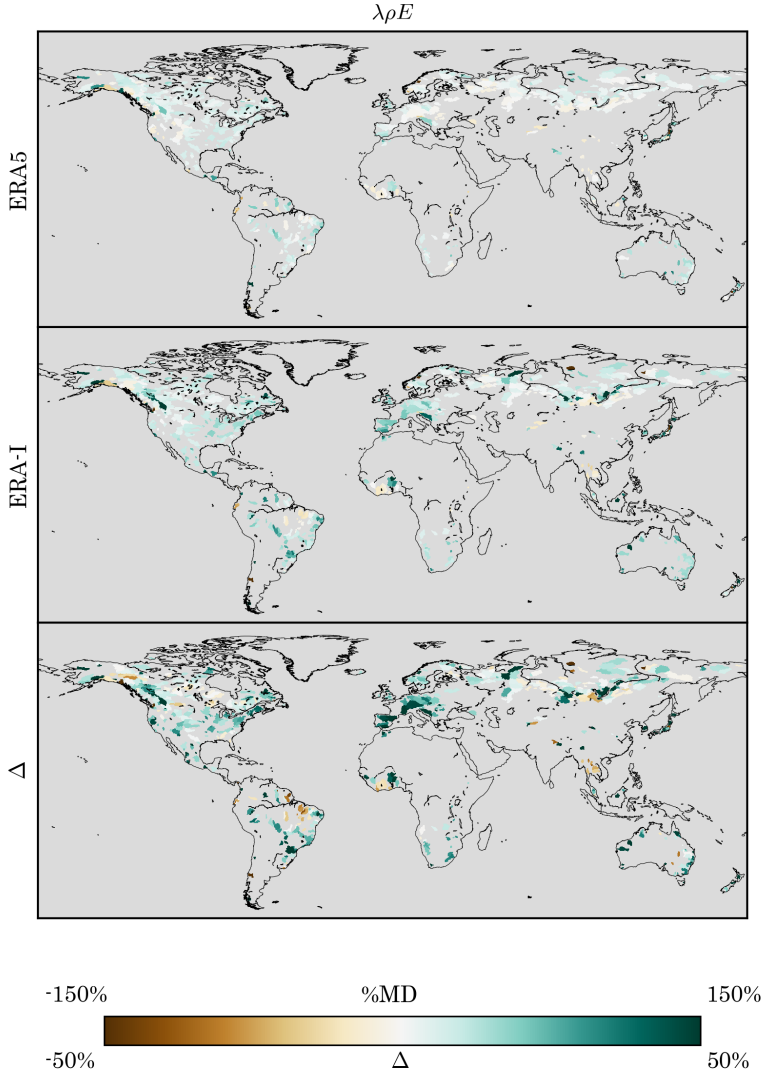


Figure 5.7: Maps of the bias of the surface latent heat flux ($\lambda\rho E$) from ERA5 and ERA-I. The bias is calculated against catchment-scale estimates of the fluxes derived using discharge data (Eqs. 5.1–5.3) and is assessed by the percentage Mean Difference (%MD, raw time series from 707 catchments as reference). The bottom map represents the difference (Δ) between the absolute value of the %MD of ERA5 and ERA-I; hence, green colors represent lower bias in ERA5 than in ERA-I.

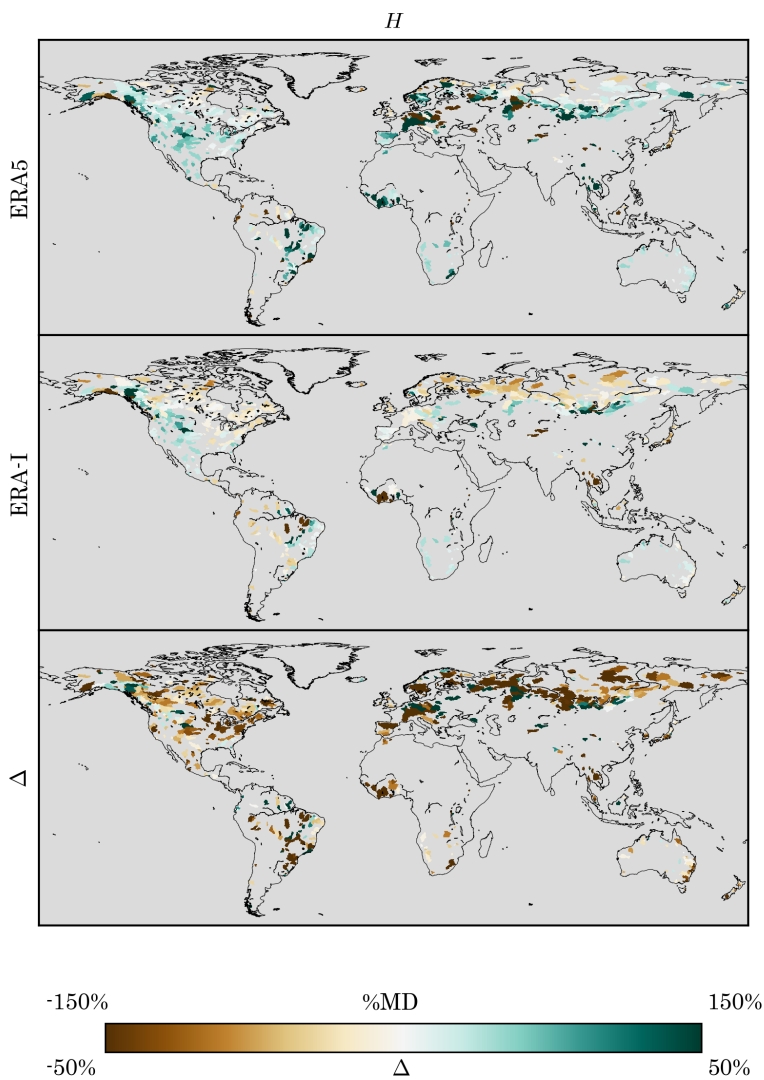


Figure 5.8: Like Figure 5.7, but for the surface sensible heat flux (H).

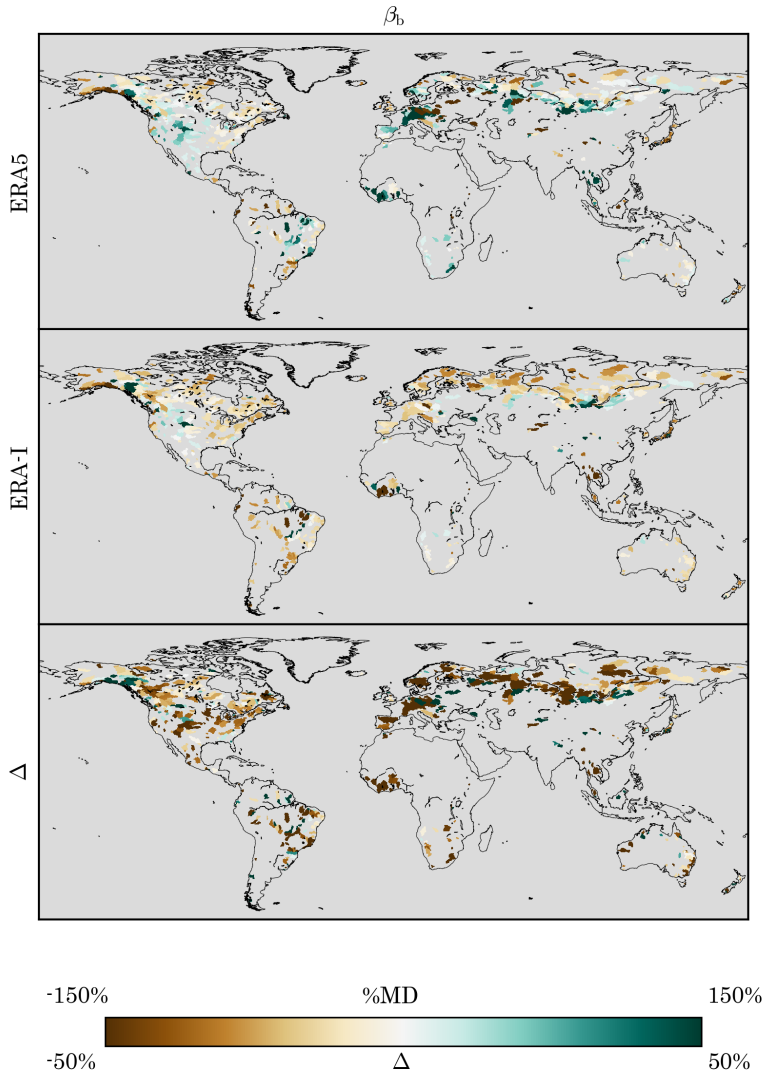


Figure 5.9: Like Figure 5.7, but for the Bowen ratio (β_b).

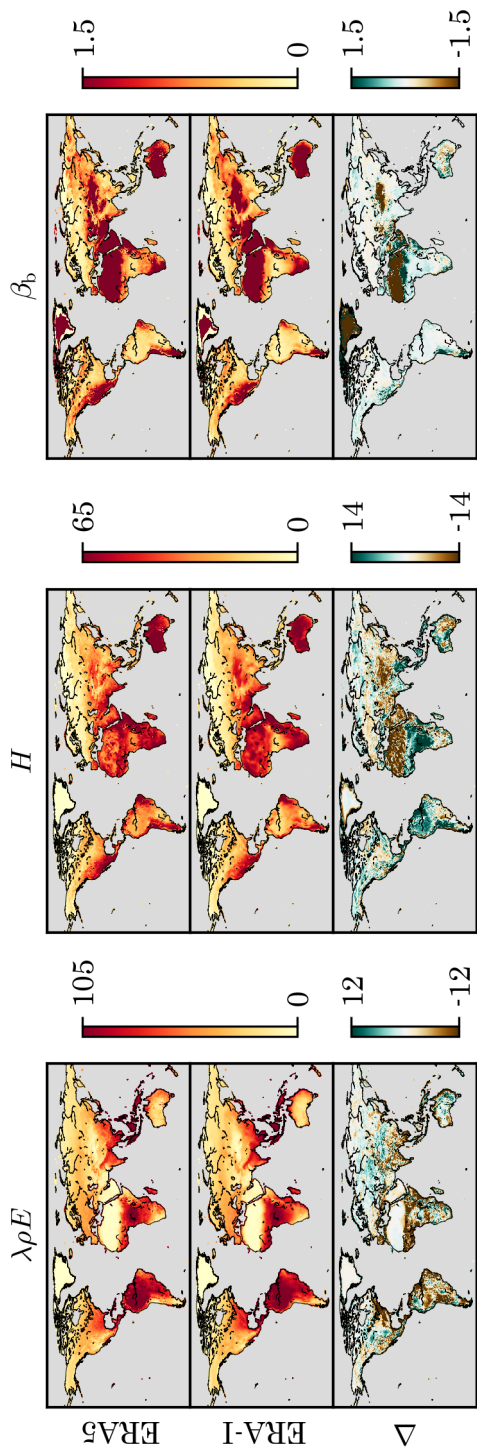


Figure 5.10: Maps of the multi-annual average of surface latent heat flux ($\lambda\rho E$, $\text{W}\cdot\text{m}^{-2}$), surface sensible heat flux (H , $\text{W}\cdot\text{m}^{-2}$), and Bowen ratio (β_b , $-$) from ERA5 and ERA-I. In the last row, Δ presents the difference between ERA5 and ERA-I; hence, green colors represent higher values in ERA5 compared to ERA-I.

The globally-averaged surface sensible heat flux from land amounts to $27.2 \text{ W}\cdot\text{m}^{-2}$ and $26.9 \text{ W}\cdot\text{m}^{-2}$ for ERA5 and ERA-I, respectively; a difference of only 1.1% (ERA-I as reference). For the surface latent heat flux, the difference is higher and sums up to -5.2% (ERA-I as reference), with global averages of $44.1 \text{ W}\cdot\text{m}^{-2}$ and $46.5 \text{ W}\cdot\text{m}^{-2}$ for ERA5 and ERA-I, respectively. The latter two values correspond to a yearly total volume of evaporated water of approximately $97.8\cdot 10^3 \text{ km}^3$ and $103.1\cdot 10^3 \text{ km}^3$. Similar values typically found in literature – although based on different land surface models or retrieval algorithms, input data sets, or region considered (e.g. areas permanently covered by snow or ice included or not) – range between $55\cdot 10^3 \text{ km}^3$ and $80\cdot 10^3 \text{ km}^3$ (Miralles *et al.*, 2016; Wang and Dickinson, 2012, and references therein), pointing towards an overestimation of the total volume of evaporated water in both ERA-I and ERA5. In terms of globally-averaged energy fluxes, the turbulent fluxes from both reanalyses lie within the uncertainty ranges reported by Wild *et al.* (2015), who inferred the magnitude of the global energy fluxes based on a detailed analysis of a variety of observations and model-based estimates. However, the surface sensible heat flux from both reanalyses can be found near the lower boundary of the interval, while the surface latent heat flux may be found near the upper limit of the interval reported in Wild *et al.* (2015). These results confirm the findings in Sections 5.3.1 and 5.3.2 and are in line with results previously reported in literature (e.g. Miralles *et al.*, 2016; Wild *et al.*, 2015; Mueller *et al.*, 2013; Jiménez *et al.*, 2011, and references therein) where similar biases were found for ERA-I.

Finally, Figure 5.10 shows that the lower globally-averaged surface latent heat flux from ERA5 mainly results from reduced values along the east coast of the CONUS, the south of Europe, the Sahel, India, and large parts of South America. These regions align well with the areas identified in Miralles *et al.* (2016) where ERA-I seemed to strongly overestimate the surface latent heat flux, and thus point to a better performance of ERA5 in these specific regions, although positive biases still prevail (Figure 5.7). The surface latent heat flux from ERA5 is higher than in ERA-I in only a few areas, such as the central CONUS, eastern Australia, and eastern Europe. For the surface sensible heat flux, differences between ERA5 and ERA-I are clearly defined, with substantially higher values in the equatorial forests and lower values in (semi-)arid regions in the case of ERA5.

5.4 Conclusion

This study evaluated the surface energy partitioning over land in ECMWF's latest reanalysis ERA5 by assessing the quality of the surface latent heat flux, surface sensible heat flux, and Bowen ratio at different spatio-temporal scales and using different validation approaches. Results were also compared with

the predecessor ERA-I for reference. Different independent in situ validation data sets – including eddy-covariance and river discharge data – were used to validate the reanalysis fields, and GLEAM was adopted as a modelling tool to assess the surface energy partitioning in both reanalyses.

In a first experiment, the turbulent fluxes and the Bowen ratio from the reanalyses were directly compared against eddy-covariance measurements from the FLUXNET 2015 data set. The analysis revealed that ERA5 performed consistently better than ERA-I for all variables analysed, both at daily and sub-daily temporal resolutions, resulting in lower MAD_{san} and higher R_{san} against in situ data. The differences were most clear when standardised anomaly time series were analysed, indicating that – although statistics also improved in case of the raw time series – ERA5 is substantially better capturing the response of surface energy partitioning to specific meteorological events. As one of the key changes in ERA5 is the use of the state-of-the-art H-TESSEL land surface model, an important part of the improvements may be attributed to the improved land parameterisation. However, a validation of some key meteorological variables against in situ measurements also showed better quality of the variables from ERA5 than from ERA-I. These results were largely confirmed by an experiment where GLEAM was forced with meteorological fields retrieved from both reanalyses, showing a higher quality of the output based on ERA5 forcing data. Finally, although ERA5 did not seem to perform particularly better than ERA-I in specific climates, it was shown that GLEAM forced with ERA5 meteorology performed better than ERA5 in terms of estimating the surface latent heat flux in warm and dry regimes, indicating possible shortcomings of H-TESSEL to capture the response of surface energy partitioning to heat and drought stress in ERA5.

In a second experiment, catchment-scale turbulent fluxes derived using discharge, precipitation, net radiation, and ground heat flux data were used to verify the bias in the annual turbulent fluxes from ERA-I and ERA5. Here, a substantial overestimation of the surface latent heat flux from ERA-I became evident. In contrast, the surface sensible heat flux appeared generally underestimated. While the biases in ERA5 for the surface latent heat flux were found to be lower – a strong reduction was found along the east coast of the CONUS and in the south of Europe – a general tendency to overestimate the latent heat flux still remains in ERA5. In case of the surface sensible heat flux, the sign of the bias reversed (i.e. in ERA5 the flux tends to be overestimated) and increased in absolute value.

Finally, the global patterns of the turbulent fluxes and Bowen ratio were analysed, and the globally-averaged magnitude of the fluxes was compared with values reported in literature. While the spatial patterns are realistic in both data sets, and align with the expectations from the major hydro-climatological regions, the substantial overestimation of the surface latent heat flux in both

reanalyses emerged again. However, the global-scale magnitude of the surface latent heat flux was found to be about 5% lower in ERA5 than in ERA-I, pointing towards the reduction of the bias, while the surface sensible heat flux only increased approximately 1%. The main reductions in the surface latent heat flux were found in regions that had previously been highlighted in literature as hotspots of overestimation in ERA-I, such as the south of Europe, the Sahel, India, large parts of South America, and the east coast of the CONUS.

In summary, based on the validation data and tools used in this study, the quality of the turbulent fluxes (and near-surface meteorology) from ERA5 shows a higher accuracy upon its predecessor. Although biases (especially in the surface latent heat flux) still prevail, changes in the IFS from ERA-I to ERA5, and improvements in the observational data sets that are assimilated into the models, have thus generally resulted in a higher-quality surface energy partitioning in the reanalysis.

On the response of terrestrial evaporation to major modes of climate variability

In this chapter, the response of terrestrial evaporation to sixteen major modes of internal climate variability is analysed. To this end, a simple supervised learning algorithm – the Least Absolute Shrinkage and Selection Operator – is used to relate dynamics in terrestrial evaporation to climate indices describing the modes of climate variability. The impact of these same modes on the local drivers of terrestrial evaporation – such as precipitation and net radiation – is also analysed to disentangle their effect on terrestrial evaporation through the modes of internal climate variability. Overall, the approach allows to define hotspots where dynamics of terrestrial evaporation are significantly driven by modes of internal climate variability, which might help to improve the representation of surface fluxes and their dynamics in Earth system models and forecasts of hydro-meteorological extremes. This chapter is an edited version of the following scientific publication:

Martens, B., Waegeman, W., Dorigo, W.A., Verhoest, N.E.C., Miralles, D.G., 2018. Terrestrial evaporation response to modes of climate variability. *npj Climate and Atmospheric Science* 1 (1), 43.

6.1 Introduction

Intra-annual and decadal variability in Earth’s climate is largely driven by large-scale and periodic changes in the (coupled) state of ocean and atmosphere, such as ENSO. These modes of climate variability do not only affect meteorological conditions in regions where they occur, but can also influence weather patterns in remote areas, being commonly referred to as teleconnections (Wallace and Gutzler, 1981). As such, modes of climate variability are expected to affect the general dynamics of ecosystems and bio-geochemical cycles inland through their impact on the local meteorological conditions driving these cycles (Claessen *et al.*, 2019; Papagiannopoulou *et al.*, 2017; Nemani, 2003). Hence, terrestrial evaporation is expected to be influenced by these teleconnections in an indirect way as well (Miralles *et al.*, 2014).

The skill of Earth system models to predict future changes in the global water cycle relies on our ability to provide insights on the response of land ecosystems to internal climate variability (Zhu *et al.*, 2017; Gonsamo *et al.*, 2016; Miralles *et al.*, 2014; Stocker *et al.*, 2013; Trenberth, 2011). As such, quantifying the sensitivity of terrestrial evaporation to the dominant modes of climate variability – and understanding the mechanisms through which these modes affect the flux – is critical to disentangle the effects of climate change on hydrology (Zhu *et al.*, 2017; Gonsamo *et al.*, 2016; Miralles *et al.*, 2014; Stocker *et al.*, 2013; Trenberth, 2011). Some studies have investigated the effect of specific teleconnections on hydroclimatological variables such as precipitation (Zhang *et al.*, 2017, 2015), temperature (Meehl *et al.*, 2016), river discharge (Emerton *et al.*, 2017; McGregor, 2017), and soil moisture (Bauer-Marschallinger *et al.*, 2013). Others have also highlighted the link between teleconnections and general ecosystem dynamics at the global scale (Zhu *et al.*, 2017; Gonsamo *et al.*, 2016). However, the response of terrestrial evaporation at global scales remains to a large degree unknown. Yet, a few studies have linked intra-annual variability in terrestrial evaporation to climate oscillations, but only at the regional scale and focussing on specific teleconnections relevant for the area of interest (e.g. Xing *et al.*, 2016; Hidalgo *et al.*, 2005).

Only recently, the emergence of global-scale, long-term data sets of terrestrial evaporation – derived from satellite and in situ data – has enabled a global analysis of the intra-annual variability in terrestrial evaporation and its link to large-scale modes of climate variability (Zhang *et al.*, 2016a, 2015; Miralles *et al.*, 2014). The study by Miralles *et al.* (2014) showed a strong control of ENSO over terrestrial evaporation in Australia, southern Africa, and eastern South America. Anomalously low volumes of evaporation in these regions during El Niño were related to rainfall deficits in these areas, resulting in higher evaporative stress and thus lower evaporation rates. In fact, ENSO is often considered to be the primary mode of internal climate variability for many regions on Earth (Trenberth, 2019; McPhaden *et al.*, 2006). However, the

overall effect of other fundamental modes on global terrestrial evaporation has not yet been explored. In addition, the dominant effect of ENSO is presumably concentrated in the tropics and the Southern Hemisphere (Miralles *et al.*, 2014), while in the Northern Hemisphere, weather patterns and ecosystem functioning are likely to be influenced by other teleconnections (Zhu *et al.*, 2017; Wallace and Gutzler, 1981). Therefore, a direct analysis of the effect of teleconnections on terrestrial evaporation is still missing, which hampers the ability to analyse the effects of internal climate variability on the global hydrological cycle (Yeh and Wu, 2018).

In this chapter, the impact of different leading modes of internal climate variability on global terrestrial evaporation is analysed. Therefore, an error-based merger of observational data sets based on GLEAM (Chapters 2 and 3), the Penman-Monteith-Leuning (PML) model (Zhang *et al.*, 2016a), and the Model Tree Ensemble (MTE; Jung *et al.*, 2011, 2009) is used. A simple supervised learning algorithm, called the Least Absolute Shrinkage and Selection Operator (LASSO; Tibshirani, 1996), is used to relate the temporal variability in the evaporative flux, and that of its local climatic drivers, to climate indices (CIs) specifically designed to diagnose the modes of climate variability. This approach allows us to disentangle the influence of inter-dependent and cross-correlated processes (Stocker *et al.*, 2013; Quadrelli and Wallace, 2004). Ultimately, the objectives are to identify the dominant modes of climate variability controlling terrestrial evaporation dynamics across the globe, and to find the local climatic drivers through which these modes act upon evaporation. The chapter is organised as follows: Section 6.2 describes the approach to tackle the main objective of this chapter, together with an in depth description of the statistical model and tests used. Section 6.3 provides an overview of the data sets used in this study, and Section 6.4 presents the results and discusses them in frame of recent literature. Conclusions and important findings are summarised in Section 6.5.

6.2 Methodology

6.2.1 General approach

A three-step approach is used to disentangle the effect of the major modes of climate variability on terrestrial evaporation. The first step aims to identify the key modes of climate variability that dominate the temporal dynamics of terrestrial evaporation in a certain region. Given that changes in the state of ocean and atmosphere drive changes in surface meteorology, subsequently affecting ecosystem functioning (and thus terrestrial evaporation), such a direct analysis in principle bypasses the need to first investigate the link between climate variability and surface meteorology on the one hand, and surface meteorology and terrestrial evaporation on the other hand. In the next two

steps, however, these two links are also assessed. As such, in the second step, the main climatic driver of terrestrial evaporation is inferred, allowing to hypothesise through which climatic driver the selected modes from the first step may be acting upon terrestrial evaporation. The third step confirms whether the modes that were identified in the first step actually impact the climatic drivers of terrestrial evaporation in a certain region. Altogether, not just the dominant modes of climate variability controlling terrestrial evaporation are identified, but also the local climatic drivers through which these modes act upon evaporation.

In each step, a statistical model is fitted for each grid cell in the target data set to disentangle the relation between the variable of interest (target variable) and potential explanatory variables (features). In the first step, the aim is to analyse the impact of sixteen modes of climate variability, diagnosed by CIs (Section 6.3), on terrestrial evaporation. Hence, statistical models are fitted targeting terrestrial evaporation (target variable) using the CIs diagnosing the modes of climate variability as predictive features. The response time of the local climatic drivers of terrestrial evaporation (and thus evaporation itself) to variations in the state of ocean and atmosphere is a priori unknown and is expected to range between 0 and 8 months (personal communication with Trenberth, K.E. on December 14, 2017). To account for this unknown response time, time lags ranging from 0 (i.e. no lag between target and CI) to 8 months (i.e. the target lags 8 months behind the CI) are introduced to each of the CIs, resulting in 144 predictive features in total (i.e. 16 CIs x 9 lags/CI) for this experiment.

In the second step, the relative control over terrestrial evaporation of two local climatic drivers (i.e. precipitation and total incoming radiation) is quantified. This step allows to objectively discern regions where terrestrial evaporation is dominated by the supply of energy (incoming radiation) or rather limited by water availability (precipitation), and thus allows to hypothesise through which of these drivers the modes are actually affecting the dynamics in terrestrial evaporation. Note that total incoming radiation is used here as a proxy for the energy supply, as it is to a large extent not affected by the land surface, and thus almost independent from terrestrial evaporation itself (except through its indirect effect on temperature, humidity, and clouds; Teuling *et al.*, 2017). This is in contrast to other studies which typically use net radiation – or potential terrestrial evaporation – to define evaporation regimes. In this experiment, it is assumed that the response of terrestrial evaporation to its drivers is rather direct (i.e. within one month) and no lags are introduced in the predictive features. Hence, models are fitted between terrestrial evaporation (target variable) and two predictive features, being total incoming radiation and precipitation.

In the third step, the relation between the two climatic drivers of terrestrial

evaporation and the sixteen modes of climate variability is analysed. Therefore, statistical models are fitted targeting precipitation on the one hand, and total incoming radiation on the other hand, based on the same 144 predictive features used in the first step (i.e. the lagged CIs) as the response time of local climatic variables to the teleconnection patterns is not known here either.

Finally, as most modes of climate variability selected in this study (Section 6.3) are known to be more active during specific seasons of the year (Zhu *et al.*, 2017; Gonsamo *et al.*, 2016; Wallace and Gutzler, 1981), separate models are fitted for four three-month periods in the target data set: December–February, March–May, June–August, and September–November; roughly corresponding to Boreal winter, spring, summer, and fall, respectively.

6.2.2 Modelling framework

LASSO

Acknowledging the potential correlation between predictive features in each of the three experiments outlined in Section 6.2.1, the LASSO is selected here as a regression method, as it has proven to perform well when features are cross-correlated (Tibshirani, 1996). In addition, the LASSO has the unique property to perform both feature selection and regularisation at the same time, typically resulting in a predictive model with only a subset of the pre-selected features, which simplifies the interpretation of the final model, and avoids the need to pre-select features based on expert knowledge or alternative statistical techniques. To do so, the method shrinks the regression coefficients towards zero by aiming at finding coefficients that minimise a penalised residual sum of squares (Tibshirani, 1996) using the coordinate descent optimisation algorithm:

$$\hat{\beta} = \operatorname{argmin} \left\{ \sum_{i=1}^n \left(y_i - \beta_0 - \sum_{j=1}^p \beta_j x_{ij} \right)^2 + \omega \sum_{j=1}^p |\beta_j| \right\}, \quad (6.1)$$

where $\hat{\beta}$ is the p -dimensional vector with the estimated regression coefficients (–), n the number of training samples in the data set (–), y_i the value of the target variable in sample i (units depend on variable under consideration), p the number of features (–), x_{ij} the value of feature j in sample i (units depend on variable under consideration), and ω the regularisation parameter (–), a hyper-parameter controlling the amount of shrinkage; higher values of ω result in more shrinkage of the regression coefficients and a higher number of features that are discarded from the model (i.e. $\beta_j = 0$). The regularisation parameter is tuned here by minimizing the prediction error of the model, estimated using a 5-fold cross validation, by computing the regularisation path of the estimator.

Model evaluation

To evaluate the actual predictive power of the fitted LASSO models and infer their significance, an independent test set is required in theory. However, given the low number of samples in the data set, and high number of features (Section 6.3), prediction errors (including the error introduced by the hyperparameter tuning, hence feature selection procedure) are estimated using an external 5-fold cross validation on top of the cross validation used for hyperparameter tuning. As such, both the validation and test errors are estimated using cross validation, resulting in a nested cross-validation approach that avoids biases in the estimates of the true prediction error due to the internal feature selection procedure (Ambroise and McLachlan, 2002), while avoiding the use of an independent test set for model evaluation. The predictive power of the fitted models is expressed here in terms of explained variance (R^2) calculated as:

$$R^2 = 1 - \frac{\text{RSS}}{\text{TSS}}, \quad (6.2)$$

where RSS is the Residual Sum of Squares calculated using the nested 5-fold cross-validation and TSS is the Total Sum of Squares (i.e. the variance of the target variable).

R^2 values are tested for statistical significance (at the 5% significance level) by comparing the empirical distribution of the sample (i.e. all values obtained across the global domain) against its analogue representing the null hypothesis of no predictive power. The null distribution of the R^2 of a LASSO model without any predictive power is obtained using a non-parametric permutation test (Good, 2004). Therefore, for each experiment described above, all LASSO models are fitted again on a random training data set, obtained by shuffling the original predictive features in time. The null distribution is then non-parametrically described by the obtained R^2 values, and compared to the analogue of the original experiment. As many hypotheses (i.e. all R^2 values across the globe) are tested at the same time, and the probability of false discoveries increases with the number of hypotheses tested (Benjamini and Hochberg, 1995), the Benjamini-Hochberg procedure (Benjamini and Hochberg, 1995) is used to control the false discovery rate at a level of 5% in this multiple hypothesis testing problem.

Feature ranking

The sensitivity of any target variable (i.e. either evaporation, precipitation, or radiation; depending on the experiment) to one of the features can be obtained by analysing the magnitude of the corresponding regression coefficient (Equation 6.1). As such, an importance ranking of the features per grid cell can be made based on the absolute values of the regression coefficients in the fitted

model. However, note that regression coefficients cannot be compared among grid cells due to the fact that different regularisation is applied (and regression coefficients are thus differently forced towards zero), as the ω parameter is optimised per grid cell (Equation 6.1). Therefore, the ranking of features (rather than their regression coefficient) will be used here to compare their impact across regions. To account for the lagged features introduced in some experiments, regression coefficients are summed over all lags per feature to obtain the overall impact of a particular feature on the target variable prior to the ranking.

Given that the modes of climate variability typically affect climatic conditions – and presumably terrestrial evaporation – across extended regions, areas with a consistent impact of certain teleconnection patterns are visually delineated and the dominant modes inferred. The former is done by analysing the global maps of the regression coefficients and the significance of the fitted LASSO models as appraised by their explained variance to only focus on regions where a significant impact is found, further referred to as hotspots. The latter is achieved by calculating for each feature the average rank over all grid cells in the hotspot.

6.3 Data

Global data sets of terrestrial evaporation, precipitation, and total incoming radiation are constructed for the period 1982–2012. All data sets are linearly resampled from their native spatial resolution to a common 0.5° latitude-longitude grid, being the coarsest spatial resolution of all selected data sets, and aggregated to a monthly temporal scale. To avoid spurious results due to similar seasonal patterns, the raw data are converted into monthly, standardised, and de-trended anomalies by (1) subtracting the multi-annual monthly average for each month of the year, (2) normalising the result by the standard deviation for that month, and (3) subtracting the linear trend from the time series per grid cell.

To obtain a robust data set of terrestrial evaporation in this study, de-trended and standardised anomalies of the GLEAM v3.1a¹, PML (Zhang *et al.*, 2016a), and FLUXNET-MTE (Jung *et al.*, 2011, 2009) global data sets of terrestrial evaporation are merged based on their relative errors calculated using a TCA (Miralles *et al.*, 2010; Scipal *et al.*, 2008; Stoffelen, 1998). The weights attributed to each of the data sets are shown in Figure C.8 (Appendix C.3). Total incoming radiation is sourced from the ECMWF ERA-I reanalysis data set (Dee *et al.*, 2011), and precipitation from MSWEP (Beck *et al.*, 2017).

¹This data set is an updated version of the v3.0a data set presented in Chapter 3. Differences include minor algorithmic updates in GLEAM and updates of the forcing data sets.

Results are thus affected by the uncertainties in these data sets. Nevertheless, both have been validated against in situ data, and compared against similar data sets in numerous studies (e.g. Beck *et al.*, 2017; Trenberth and Fasullo, 2013), and it has been concluded that both data sets are robust and reliable in terms of intra-annual variability.

The sixteen selected modes of climate variability (Table 6.1) are diagnosed by CIs, generally obtained by temporal analysis of sea-surface temperature or geo-potential height fields in specific regions or points on Earth. These indices provide a simple statistical summary of complex and inter-related processes resulting in the modes of internal climate variability (Kingston *et al.*, 2006). CIs are obtained from various centers from the National Oceanic and Atmospheric Administration (NOAA), and the Climate Explorer of KNMI. CIs are typically correlated, as a result of the interactions between different climate phenomena impacting each of the CIs (Stocker *et al.*, 2013; Quadrelli and Wallace, 2004). This is illustrated in Supplementary Figure C.9 (Appendix C.3), which shows a correlation matrix of the sixteen CIs at lag 0 and evidences the significant dependency between some of the selected CIs, supporting the choice for the LASSO as a regression method (Section 6.2.2).

Table 6.1: Selected modes of climate variability and their corresponding CI obtained from various centers from the National Oceanic and Atmospheric Administration, and the Climate Explorer of KNMI.

Mode of variability	CI
Atlantic Meridional Mode (AMM)	AMM sea-surface temperature index
Atlantic Multidecadal Oscillation (AMO)	AMO index
East Atlantic Pattern (EA)	EA index
East Atlantic West Russia Pattern (EAWR)	EAWR index
East Pacific North Pacific Pattern (EPNP)	EPNP index
El Niño Southern Oscillation (ENSO)	Southern oscillation index
Indian Ocean Dipole (IOD)	Dipole mode index
Northern Annular Mode (NAM)	NAM index
North Atlantic Oscillation (NAO)	NAO index
Pacific Decadal Oscillation (PDO)	PDO index
Pacific-North American Pattern (PNA)	PNA index
Polar Eurasia Pattern (PEA)	PEA index
Southern Annular Mode (SAM)	SAM index
Tropical Northern Atlantic Dipole (TNA)	TNA index
Tropical Southern Atlantic Dipole (TSA)	TSA index
West Pacific Pattern (WP)	WP index

6.4 Results and discussion

Figure 6.1a shows that monthly evaporation anomalies are significantly (at the 5% significance level) driven by the main modes of climate variability in about half of the land surface. Clear hotspots where up to 40% of the variance in

terrestrial evaporation can be explained by the CIs can be identified for different seasons (Figure 6.1b). In these seasonal hotspots, terrestrial evaporation is typically sensitive to a limited number of modes, suggesting both the control of these modes over the local meteorology, and the control of the latter over evaporation. Below, the main hotspots that can be observed in Figure 6.1 are briefly described and observed patterns are benchmarked against results found in recent literature.

6.4.1 Southern Hemisphere and tropical hotspots

Figure 6.1b shows that throughout the year, variability in terrestrial evaporation in Amazonia is influenced by multiple teleconnections: although ENSO is identified as an important driver of variability in December–February in the east, and in March–May in the south, evaporation dynamics in the rainforest are also sensitive to the Indian Ocean Dipole (IOD) pattern, the Atlantic Multi-decadal Oscillation (AMO), the Pacific Decadal Oscillation (PDO), and the Tropical North Atlantic (TNA) pattern. During June–August, the TNA has also a distinct effect in the arc of deforestation (i.e. south of the Brazilian rainforest).

Given the high volumes of precipitation in these regions, dynamics in terrestrial evaporation are primarily driven by variations in energy supply, as shown in Figure 6.2. Recall that total incoming radiation is used here as a proxy for the energy supply (Section 6.3), as it is to a large extent not affected by the land surface (and thus terrestrial evaporation). However, results using surface net radiation show similar patterns as shown in Figure C.10 (Appendix C.3), and are comparable to maps published in literature (e.g. Seneviratne *et al.*, 2010).

Rainfall interception loss also forms a substantial portion of the total evaporative flux in the rainforest (Martens *et al.*, 2017; Miralles *et al.*, 2011a), making Amazonian evaporation sensitive to changes in rainfall dynamics as well. The sensitivity of rainfall interception loss to ENSO due to its influence on precipitation variability was already documented by Miralles *et al.* (2014). Figure 6.3 shows that this mechanism mostly explains the impact of ENSO in the northeast of the rainforest during December–February (Supplementary Figure C.15, Appendix C.3), but not for the arc of deforestation where rainfall dynamics are not affected. In the latter, the impact of ENSO and TNA on evaporation comes from their influence on the energy supply (Figure 6.3 and Supplementary Figures C.20 and C.21, Appendix C.3), mostly due to changes in air temperature and cloud cover. Note that ENSO is also known to induce substantial variability in tropical Atlantic sea-surface temperatures, driving the TNA and Tropical South Atlantic (TSA) patterns that in turn alter the meteorology in the northeast of Brazil (García-Serrano *et al.*, 2017; Enfield and Mayer, 1997) as shown in Supplementary Figures C.17 and C.18 and

Supplementary Figures C.21 and C.22 (Appendix C.3). Finally, the multi-decadal AMO typically modulates the intensity of the ENSO cycle (Baek *et al.*, 2017; Vásquez *et al.*, 2017), hence the effect of AMO on evaporation in Amazonia is presumably indirect.

In the southwestern Pacific, ENSO, IOD, AMO, and the Southern Annular Mode (SAM) influence terrestrial evaporation during June–August and September–November (Figure 6.1b), especially in the east of Australia, a semi-arid region where terrestrial evaporation is mainly driven by water availability (Figure 6.2). Results in Figure 6.3 show that in June–August, precipitation in central east Australia is affected, mainly by SAM and ENSO (Supplementary Figure C.17, Appendix C.3). In contrast, the hotspot in September–November is due to a combined effect on the water and energy supply induced by ENSO and SAM (Supplementary Figure C.18, Appendix C.3), and particularly by the effect of IOD on the energy supply in the southeast (Supplementary Figure C.22, Appendix C.3). This sensitivity of evaporation to ENSO in east Australia is in agreement with the findings in Miralles *et al.* (2014), while Bauer-Marschallinger *et al.* (2013) pointed to the relation between the IOD and soil moisture dynamics in Australia, which can be linked to the results discussed here. A positive phase of the IOD also typically results in wet anomalies in the Horn of Africa (Bauer-Marschallinger *et al.*, 2013) as indicated in Supplementary Figure C.15 (Appendix C.3), which explains the hotspot in December–February shown in Figures 6.1b and 6.3.

6.4.2 Northern Hemisphere hotspots

In contrast to the Southern Hemisphere, the effect of individual modes of climate variability in the Northern Hemisphere is generally concentrated to specific regions. This confined effect is in agreement with the findings by Zhu *et al.* (2017) on the impact of teleconnections on global carbon fluxes. In northwestern Europe, wintertime terrestrial evaporation is shown to be sensitive to modes of variability known to modulate the European winter climate: the North Atlantic Oscillation (NAO) and the East Atlantic (EA) pattern (Baek *et al.*, 2017; Gao *et al.*, 2017; Steirou *et al.*, 2017; Kingston *et al.*, 2006). During December–February, evaporation dynamics in the region are not just influenced by the energy supply (Figure 6.2) but also by precipitation, due to its influence on rainfall interception (Miralles *et al.*, 2011a). The positive phase of NAO and EA typically bring more precipitation and higher temperatures to northern Europe during winter (Steirou *et al.*, 2017), as confirmed in Supplementary Figures C.15 and C.19 (Appendix C.3), which explains the impact of these modes on terrestrial evaporation shown in Figure 6.1b. At the same time, negative precipitation anomalies typically occur in the south of Europe during the positive phase of NAO (Steirou *et al.*, 2017) as shown in Supplementary Figure C.15 (Appendix C.3), which lead to a decline in evaporation in this

water-driven region (Figure 6.2), and explains the small hotspot along the west coast of Portugal shown in Figure 6.1b (not highlighted, but statistically significant). Figure 6.3 shows that more towards the center of the European continent, the energy supply during winter is affected, mainly by both NAO and EA (Supplementary Figure C.19, Appendix C.3), thereby the influence of these teleconnection patterns on evaporation shown in central Europe.

In eastern Europe and western Russia, the East Atlantic Western Russia (EAWR) pattern starts affecting evaporation dynamics in March–May in the north, and gradually becomes more dominant in summertime (Figure 6.1b). Figure 6.3 shows how the available energy, driving terrestrial evaporation during that time of the year (Figure 6.2), is clearly impacted by the EAWR (Supplementary Figure C.21, Appendix C.3). These findings agree with those by Ionita (2014), and indicate that the positive phase of the EAWR typically results in negative temperature anomalies over eastern Europe and western Russia (Supplementary Figures C.20–C.21, Appendix C.3), resulting in the negative anomaly in terrestrial evaporation observed in Figure 6.1b. In the northeast of Russia, terrestrial evaporation is mainly sensitive to the IOD, and the West Pacific (WP) and East Pacific/North Pacific (EPNP) patterns. Both the WP and EPNP induce substantial variability in air temperatures across the region (Baxter and Nigam, 2015; Linkin and Nigam, 2008; Wallace and Gutzler, 1981), resulting in anomalies in the energy supply (Figure 6.3 and Supplementary Figures C.20 and C.21, Appendix C.3), which propagate to the dynamics in terrestrial evaporation.

In North America, terrestrial evaporation responds to various modes of variability, with the EPNP, NAO, WP, the Northern Annular Mode (NAM), and the Pacific-North American (PNA) pattern being the most dominant ones, depending on the region considered. Figure 6.1b shows that the EPNP pattern affects evaporation dynamics in the area surrounding the Great Lakes in September–May. The impact of the EPNP on evaporation in North America is opposite to its impact in Siberia (Supplementary Figures C.11–C.14, Appendix C.3). This is due to the contrasting effects of the EPNP on the energy supply in both areas (Supplementary Figures C.19–C.22, Appendix C.3). Figure 6.1b also shows that the Labrador Peninsula is largely influenced by NAO and NAM in December–May, with negative anomalies in evaporation associated with a positive phase of NAO and NAM (Supplementary Figures C.11–C.12, Appendix C.3). This effect is driven by the impact of NAO and NAM on the supply of energy in the region, as shown in Supplementary Figures C.19 and C.20 (Appendix C.3). NAO is sometimes considered as a regional-scale expression of the large-scale NAM, both having analogous climatological impacts in North America (Steirou *et al.*, 2017; Hurrell and Deser, 2009; Kingston *et al.*, 2006). The positive phase of NAO and NAM also results in higher temperatures southwards, along with positive radiation anomalies at the East Coast of the

United States (Hurrell and Deser, 2009; Kingston *et al.*, 2006), as illustrated in Supplementary Figure C.19 (Appendix C.3). Despite the strong energy control over terrestrial evaporation in this region (Figure 6.2), the impact of NAO and NAM on evaporation appears lower and is not highlighted in Figure 6.1b. The PNA is mainly affecting evaporation in the Canadian Prairies: higher evaporation is associated with the positive phase of the PNA during the winter months (Figure 6.1b), due to the impact of PNA on the energy supply in the region (Figure 6.3 and Supplementary Figure C.19, Appendix C.3).

Finally, the hotspot in the southwest of the United States and, particularly Mexico, is primarily affected by ENSO, TSA, and SAM (Figure 6.1b). Given the low precipitation volumes in the area, evaporation dynamics are mainly water-driven (Figure 6.2). However, only ENSO leads to substantial changes in precipitation, preferentially in wintertime (Supplementary Figure C.15, Appendix C.3), while the remaining modes act upon evaporation by affecting the atmospheric demand for water as shown in Supplementary Figures C.19 and C.20 (Appendix C.3). During the warm phase of ENSO (i.e. El Niño), the area typically receives more precipitation (Baek *et al.*, 2017) as indicated by Supplementary Figure C.15 (Appendix C.3), resulting in less evaporative stress and positive anomalies in terrestrial evaporation (Miralles *et al.*, 2014).

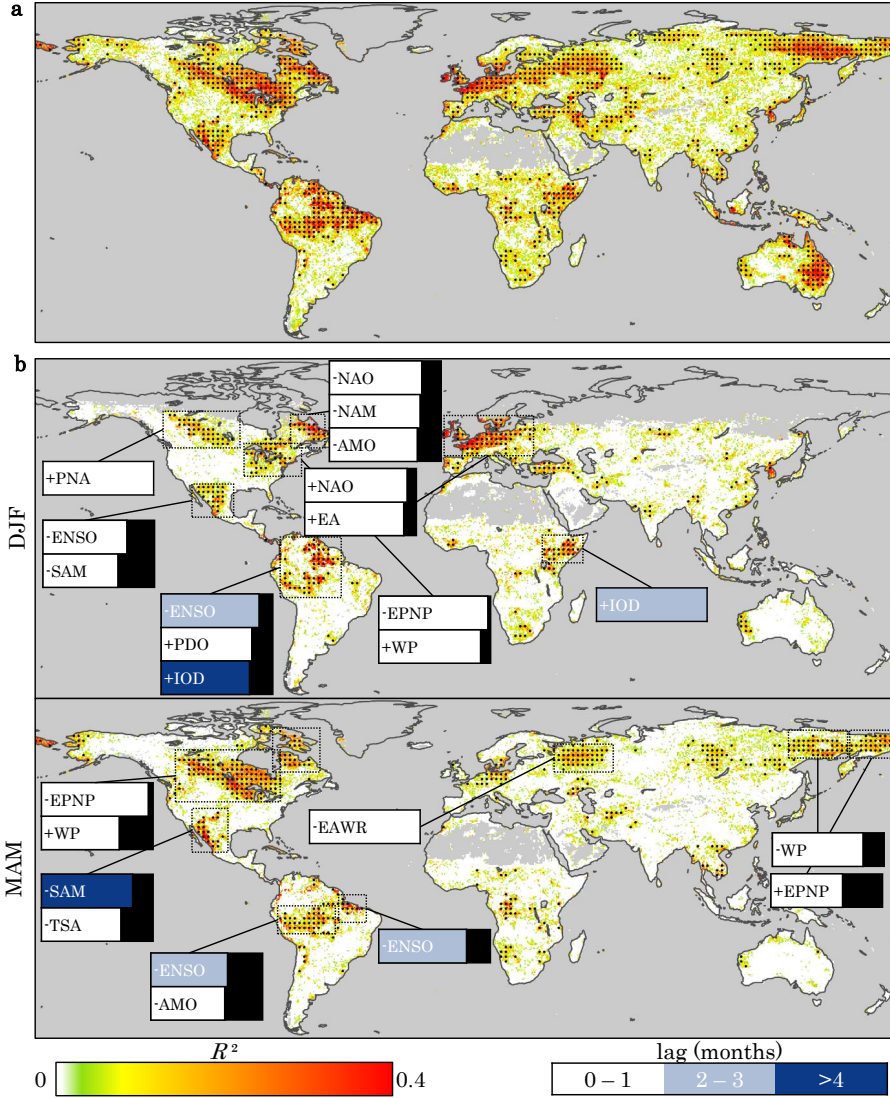


Figure 6.1: Impact of teleconnections on terrestrial evaporation. (a) Maximum explained variance (R^2) of the LASSO models targeting terrestrial evaporation based on the CIs over each season, and (b) the R^2 for the models fitted for December-January-February (DJF), March-April-May (MAM), June-July-August (JJA), and September-October-November (SON) separately. The net of dots is presented at a 2° grid to aid visibility, and indicates statistically significant R^2 (at the 5% significance level). Teleconnections dominating the variability in terrestrial evaporation are listed according to their average rank in the hotspots, represented by the length of each box (dark box in the background represents the highest possible rank; i.e. the mode is ranked first in every grid cell of the hotspot). Ranking is based on the magnitude of the regression coefficients in the LASSO model. The sign indicates the relation between the CI and evaporation (Supplementary Figures C.11–C.14, Appendix C.3), and the blue shades indicate the lag (in months) between the CI and the impact on evaporation.

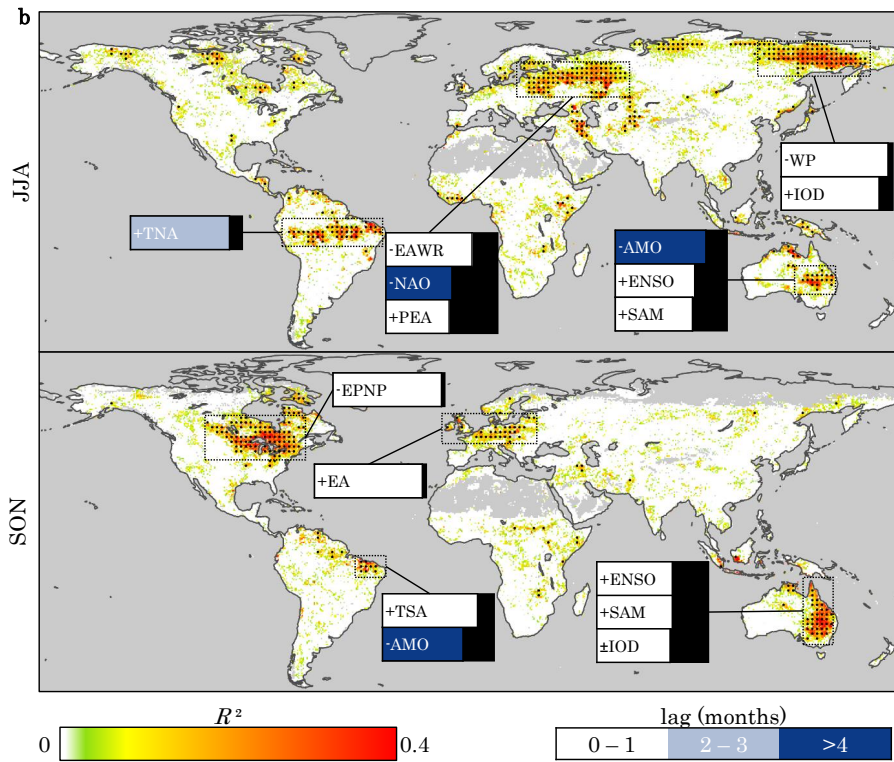


Figure 6.1: Maps showing the impact of teleconnections on terrestrial evaporation at the global scale (continued).

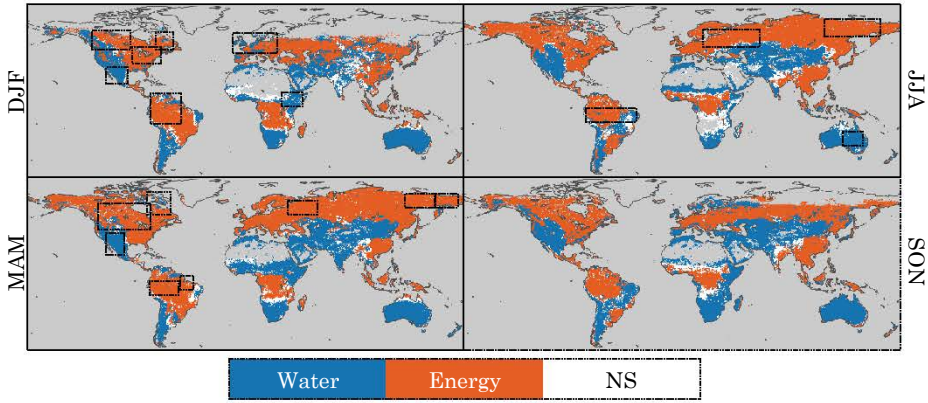


Figure 6.2: Primary climatic driver of terrestrial evaporation. Classification is obtained by ranking the regression coefficients from the LASSO model targeting the anomalies of terrestrial evaporation based on the anomalies of precipitation and total incoming radiation. Grid cells where the regression coefficient for precipitation is top-ranked are classified as water-driven, whereas grid cells where the regression coefficient for radiation is top-ranked are classified as energy-driven. NS indicates non-significant grid cells. For comparison, the regions of interest were aligned with the ones in Figure 6.1.

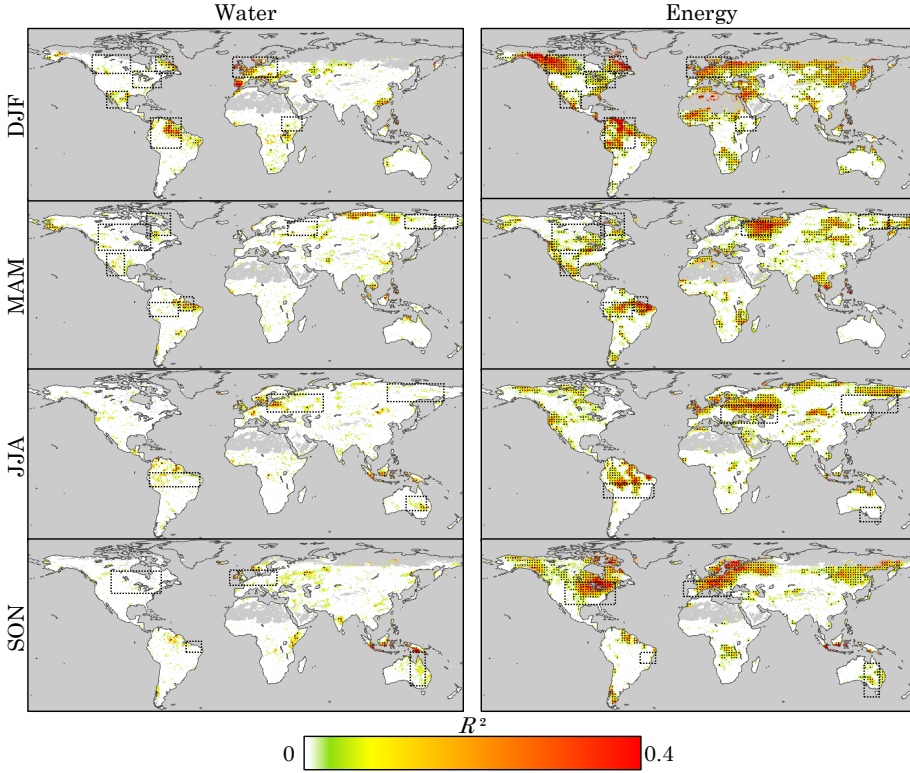


Figure 6.3: Dependence of the primary drivers of terrestrial evaporation on teleconnections. R^2 of the LASSO models targeting the anomalies of precipitation (water), and total incoming radiation (energy) based on the CIs for December-January-February (DJF), March-April-May (MAM), June-July-August (JJA), and September-October-November (SON) separately. The net of dots is presented at a 2° resolution to aid visibility, and highlights regions with a statistically significant R^2 (at the 5% significance level). For comparison, the regions of interest were aligned with the ones in Figure 6.1.

6.4.3 General discussion

Figure 6.3 shows that while precipitation patterns are sensitive to the fundamental modes of climate variability in rather confined areas, total incoming radiation is impacted world-wide. This suggests that most modes affect terrestrial evaporation through altering the atmospheric demand for water (i.e. they affect the incoming radiation through e.g. the occurrence of clouds). This particularly applies to areas and seasons in which water availability is not limiting the evaporative flux, like northern Europe, Russia, east of North America, and the equatorial belt (Figure 6.2). Nonetheless, changes in precipitation might still affect the evaporation dynamics in these wet regions through their impact on interception loss, which represents a substantial fraction of the total evaporative flux in forested regions such as Amazonia (Martens *et al.*, 2017; Miralles *et al.*, 2011a). It should be noted that many of the Northern Hemisphere teleconnections – generally affecting the energy supply – have their primary impact during winter, especially in western Europe, which might in fact make them less important in absolute terms given the lower volumes of evaporation in winter time. In arid and semiarid regions such as Mexico, the horn of Africa, and the east of Australia, the impact of the teleconnection patterns on the energy supply is generally not affecting evaporation dynamics. When existent, the impact of the modes on terrestrial evaporation in these regions is induced by changes in water supply (Figure 6.3). Results presented in Figure 6.1b also show that the response of terrestrial evaporation to most modes of climate variability has a short latency, with average lag times ranging between zero and two months.

Overall, ENSO is found to affect evaporation dynamics in the largest portion of land (Figure 6.4). This result confirms the notion that ENSO is a dominant mode of internal climate variability, affecting a wide range of land surface processes (Trenberth, 2019; Emerton *et al.*, 2017; Zhu *et al.*, 2017; Gonsamo *et al.*, 2016; Iizumi *et al.*, 2014; Miralles *et al.*, 2014; McPhaden *et al.*, 2006). However, as shown in Figure 6.4, several teleconnections affect terrestrial evaporation over similarly extensive areas. In addition, when several modes influence evaporation concurrently, ENSO is often not the most dominant one. When considering only the dominant mode acting upon evaporation in each grid cell, AMO is by far the most important in both hemispheres. Nonetheless, given the multi-decadal periodicity of AMO, its effect on terrestrial evaporation comes mostly through its influence on other modes of climate variability such as ENSO (Baek *et al.*, 2017; Vásquez *et al.*, 2017). Also the TSA and TNA patterns dominate variability in terrestrial evaporation in relatively large regions of both hemispheres, mainly along the equatorial Atlantic (Enfield and Mayer, 1997). Except for the IOD, which also affects evaporation in both hemispheres, most other teleconnections have their dominant impact in confined areas of the Northern Hemisphere (Figure 6.4).

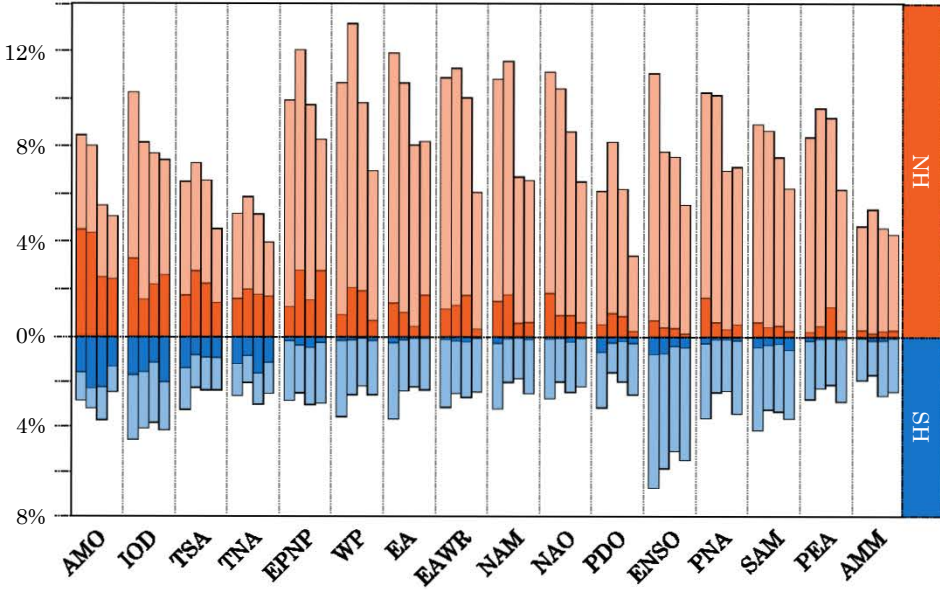


Figure 6.4: Land area subject to the influence of each teleconnection on terrestrial evaporation. Dark shades show the percentage of land area where each mode dominates the variability in terrestrial evaporation (i.e. the mode is top-ranked in the LASSO model), and light shades show the percentage of land area where each mode affects the variability in terrestrial evaporation (i.e. the oscillation has a regression coefficient > 0 in the LASSO model). Percentages are calculated relative to the total land area, excluding grid cells with missing data (e.g. in high latitudes during winter). Importance ranking is based on the magnitude of the regression coefficients from the resulting LASSO model targeting the anomalies of terrestrial evaporation based on the CIs (Supplementary Figures C.11–C.14, Appendix C.3). Only statistically significant (at the 5% significance level) models are considered. Results are shown from left to right for December-January-February (DJF), March-April-May (MAM), June-July-August (JJA), and September-October-November (SON). Modes of climate variability are ranked in this plot according to the average dominance over all seasons.

6.5 Conclusion

In this chapter, a global atlas of hotspots was derived where dynamics of terrestrial evaporation are significantly driven by the major modes of internal climate variability. To this end, a simple supervised learning method called the LASSO was adopted to build models targeting terrestrial evaporation using CIs as predictive features. In addition, a similar analysis was also performed on the local climatic drivers of terrestrial evaporation, aiming to evaluate through which drivers these climate modes are affecting the dynamics of terrestrial evaporation.

The results show that in about half of the land surface, terrestrial evaporation dynamics are significantly driven by modes of internal climate variability, mainly through their impact on the atmospheric demand for water. However, in regions where water availability is a limiting factor for terrestrial evaporation, or where interception loss plays a dominant role, climate modes may still affect evaporation dynamics through their impact on precipitation as well. Although ENSO is generally not the dominant mode, it affects dynamics in terrestrial evaporation across the largest part of the land surface.

In conclusion, our results highlight the control of the main modes of climate variability upon the return-flow of water from land to atmosphere. External climate forcing impacts the intensity and frequency of these modes (Knudsen *et al.*, 2014; Stocker *et al.*, 2013; Stevenson, 2012; Trenberth, 2011), which will have regional-dependent impacts on local water resources. More efforts to provide observational evidence on the sensitivity of global hydrology to internal climate variability – and to separate its effect from externally-induced changes – are a necessary step to benchmark Earth system models, and increase their skill to project the dynamics of our hydrosphere. In addition, such insights might substantially improve seasonal forecasts of hydrological variables and weather, as most CIs can nowadays be forecasted several months ahead with relatively high confidence (Hudson *et al.*, 2011). CIs might therefore be useful in combination with forecasts of hydrological forcing variables, such as precipitation and temperature, to guide hydrological models. As CIs typically integrate the effect of different meteorological drivers, they might even be used in isolation in a proper statistical framework, thereby bypassing the need for seasonal forecasts of the hydrological drivers. Results presented in this chapter can help guiding the selection of proper CIs to help improve these forecasts and related early-warning systems for hydro-meteorological events such as droughts and floods.

CHAPTER 7

Conclusion and outlook

7

This last chapter summarises the most important findings of this dissertation, which were discussed in detail in Chapters 2–6 and their dedicated scientific publications. This chapter also discusses current shortcomings of GLEAM and outlines a roadmap to guide its development. Finally, a non-exhaustive list of potential pathways to advance the scientific field of terrestrial evaporation monitoring is also provided.

7.1 Introduction

Terrestrial evaporation is an essential climate variable linking different biogeochemical cycles at the land surface and playing a key role in land–atmosphere feedbacks. Thereby, the flux affects the development and occurrence of droughts, the cycling of energy and moisture in the atmosphere, air temperature, cloud formation, and precipitation (Section 1.1.1). In addition, given that terrestrial evaporation is essentially a net loss of water from the land surface, it is the primary variable necessary to manage our water resources, thereby securing food and energy production, and the availability of fresh water (Section 1.1.1). Despite the fact that terrestrial evaporation can be measured (or estimated) with relatively high accuracy in the field, problems arise when information is needed over extended areas, as the flux cannot be directly observed with remote sensors mounted on drones, air planes, or satellites (Section 1.1.4). This mainly applies at the global scale, but also for local-scale applications such as agricultural planning or water resources management. Current techniques are thus incapable of providing data with the required spatio-temporal detail and accuracy. Motivated by this limitation, this work concentrated on generating state-of-the-art satellite-based and observational data sets of terrestrial evaporation at different spatio-temporal scales to aid local water-resources management, but also to enable global-scale climate studies, to help benchmarking climate models, and to support developing reanalysis data sets. More specifically, the three key objectives of this dissertation were formulated as:

1. To support global hydrological, atmospheric, and climate studies by deriving a global data set of terrestrial evaporation from satellite data at coarse spatial resolution (i.e. ± 25 km).
2. To aid local water resources management and agricultural planning by deriving a pilot data set of terrestrial evaporation for The Netherlands, Flanders, and the west of Germany from satellite data at high spatial resolution (i.e. 100 m).
3. To reveal the potential of the global data set derived in this dissertation for benchmarking climate reanalyses and to advance our understanding of the global-scale variability of terrestrial evaporation.

Striving towards meeting these objectives, a first step has been to advance GLEAM – a process-based model designed to estimate terrestrial evaporation from satellite-based observations – with the aim to derive global data sets of terrestrial evaporation at 0.25° spatial resolution (Chapters 2 and 3). In a second step, a pilot data set at 100 m spatial resolution for The Netherlands, Flanders, and the west of Germany (Chapter 4) was derived to assess the potential of GLEAM to be applied at high spatial resolution. Finally, the

multi-decadal global data set derived in Chapter 3 was used as a tool (1) to benchmark surface energy partitioning in the latest state-of-the-art climate reanalysis from ECMWF, ERA5 (Chapter 5), and (2) to investigate the multi-decadal variability of terrestrial evaporation and its link to internal climate variability at the global scale (Chapter 6). The main findings of these different studies are discussed in detail and summarised in their dedicated chapters and scientific publications. In this final chapter, an in-depth discussion of the main limitations of this work is given, the most important results of this dissertation are highlighted, and future perspectives are defined. The chapter is organised as follows: Section 7.2 summarises the results and key findings from this dissertation and links them to the objectives defined in Section 1.2. In addition, Section 7.2 also provides a critical discussion of the main limitations and shortcomings of methods and data sets used in this dissertation. Furthermore, a roadmap is drafted to guide the development of GLEAM (Section 7.3.1), the model used in this dissertation, and potential pathways to advance the scientific field of terrestrial evaporation monitoring are provided in Section 7.3.2.

7.2 General conclusion and discussion

7.2.1 GLEAM at coarse spatial resolution

A key component of GLEAM is the water-balance model used to estimate root-zone soil moisture. The latter is an important input for the stress module that converts potential into actual evaporation. As a result, space-based observations of surface soil moisture present a valuable means to improve the estimates of GLEAM via data assimilation. In Chapter 2, the potential of surface soil moisture data assimilation to improve the estimates of root-zone soil moisture and terrestrial evaporation from GLEAM was explored. To this end, an experimental study over continental Australia was conducted where surface soil moisture retrievals from SMOS and AMSR-E were assimilated into GLEAM using a simple Newtonian Nudging algorithm. The impact of the data assimilation system was evaluated by comparing the estimates of soil moisture and terrestrial evaporation from GLEAM against a sample of in situ measurements across the continent. The experiment provided useful insights on the optimal setup for the assimilation framework, but also important understanding on the quality of both SMOS and AMSR-E observations. Hence, GLEAM was demonstrated to be a useful tool to evaluate satellite-based soil moisture retrievals.

Results described in Chapter 2 pointed out that the assimilation of surface soil moisture in GLEAM had a clear potential to improve the estimates of root-zone soil moisture, but that the impact on the estimates of terrestrial evaporation was mild. In addition, it was shown that the assimilation of satellite-based surface soil moisture often resulted in unrealistic high-frequency

fluctuations in the model output that were not present in the in situ data. While this could be partly explained by noise in the satellite-based soil moisture data sets and the representativeness mismatch between the GLEAM grid cell and in situ soil moisture measurements, it was potentially also a result of the sub-optimal configuration of the data assimilation system, or its simplicity. The Newtonian Nudging algorithm in GLEAM misses several aspects of more complex data assimilation systems, such as those from the Kalman filter family, that account for the complex error-covariance structure between the states and observations that are assimilated. While the latter techniques could potentially increase the added value of the assimilation system, they typically require a substantial amount of tuning and are more computationally demanding (Lievens *et al.*, 2017). In addition, relatively simple techniques, such as Newtonian Nudging, fall within the rationale of GLEAM to keep the method as simple and observation-driven as possible. Finally, results also indicated that the configuration of the data assimilation system explored in Chapter 2 induced seasonal biases in the estimates of GLEAM as a result of the simple bias-correction approach used in that chapter. This issue needed particular attention and was further tackled in Chapter 3.

An important limitation of the validation approach that arose from the analyses presented in Chapter 2, but also in Chapters 3–5, was the limited availability of in situ validation data. In addition, the available data was generally not uniformly distributed across the study domain resulting in the under-representation of certain hydro-climatological regimes such as tropical and boreal forests. While this was the case for the in situ soil moisture data, it was certainly an issue for the eddy-covariance data used throughout this dissertation. Hence, results should be interpreted with care and not extrapolated to regions where in situ data are limited, or regimes that were not represented well in the original validation data set. Another important issue with the eddy-covariance data used in this dissertation was the fact that the technique tends to underestimate the latent heat flux as described in Section 1.1.3. However, correcting this underestimation requires the availability of in situ measurements of net radiation and the ground heat flux to close the energy balance, data that were not routinely available at every in situ site. Finally, the in situ measurements used in this thesis could be considered as point-scale data as compared to the spatial resolution of the models in Chapters 2, 3, and 5. Validation metrics calculated against these measurements thus partly capture errors that are not necessarily due to shortcomings in the models, but also due to a representativeness mismatch between the model grid cell and the spatial support of the in situ measurement. Despite the limitations of the validation data used in this dissertation, the eddy-covariance approach is considered to be one of the most accurate techniques to measure the surface turbulent fluxes (Section 1.1.3) and was thus preferred here as primary reference

data set. In addition, the FLUXNET 2015 data set is available in a common data format, and data are processed with consistent software and standardised methods, making the data set particularly interesting to be used in large-scale studies.

Aiming at further improving the estimates of GLEAM – and pursuing a more in-depth evaluation of the model – three major modifications were introduced in GLEAM and evaluated using a global-scale data set of in situ measurements in Chapter 3. These changes mainly focused on an improved representation of evaporative stress and included: (1) revised empirical functions to estimate evaporative stress from root-zone soil moisture and VOD, (2) an optimised water-balance model to estimate root-zone soil moisture, and (3) an advanced soil moisture data assimilation system based on insights from Chapter 2. Given the substantial impact of these modifications, a new version was developed (GLEAM v3) and data sets derived using this model were made publicly available using www.gleam.eu (last visit: 18 November 2019) as a gateway.

The advances in GLEAM were evaluated using a validation data set composed of measurements from 91 eddy-covariance towers and 2325 soil moisture sensors distributed worldwide. Based on a comparison of validation statistics for GLEAM v3 and GLEAM v2, it could be concluded that the new version of GLEAM was performing substantially better than its predecessor in terms of soil moisture dynamics. Unfortunately, the impact of the modifications on the quality of terrestrial evaporation could not be revealed unambiguously by the in situ validation. Despite the use of a large sample of in situ evaporation measurements in Chapter 3, as compared to the analyses in Chapter 2, the sample was not uniformly distributed across climatological regimes, potentially masking important differences between both versions of GLEAM. Another important limitation of the analyses in Chapter 3 was the fact that the partitioning of terrestrial evaporation into its components could not be validated against in situ data. Despite that different modifications in GLEAM – like the updated stress module (Section 3.2.3) and the use of the high-resolution land cover fractions (Section 3.3.1) – have an impact on this partitioning, it could not be objectively investigated due to the very limited availability of actual in situ validation data (Stoy *et al.*, 2019; Talsma *et al.*, 2018a). However, overall, the changes in GLEAM led to a more realistic representation of physical processes and a better quality of the data sets, particularly in the case of the root-zone soil moisture estimates.

Compared to more complex land surface models – that aim to describe the terrestrial water, carbon, and energy cycles, and their complex interactions (Section 1.1.2)– GLEAM is a relatively simple conceptual model. The model aims to maximise the use of satellite-based input data and to extract as much information as possible from these data to constrain its estimates of root-zone soil moisture and terrestrial evaporation by observations. To increase the impact

of these observations – and to keep the model applicable at global scales – many model components are intentionally kept simple and empirical, such as the stress and soil-water balance module. In addition, parameters are typically derived from literature, rather than being optimised using calibration procedures. While such empirical components might induce substantial uncertainties into the estimates of GLEAM, they keep the model applicable at global scales and at spatial resolutions currently useful for global studies. However, moving into higher spatial resolutions – such as the target resolution used in Chapter 4 – might require revising some of these model components (Section 7.2.2). Despite its apparent simplicity, GLEAM has been shown to generally perform well as compared to alternative data sets in numerous studies (e.g. Pan *et al.*, 2019; Gomis-Cebolla *et al.*, 2019; Talsma *et al.*, 2018a; McCabe *et al.*, 2016; Michel *et al.*, 2016; Miralles *et al.*, 2016; Mueller *et al.*, 2013; Jiménez *et al.*, 2011) and the new version of GLEAM introduced in Chapter 3 has been proven to produce higher quality data as compared to its predecessor. Nevertheless, GLEAM can be further advanced in several ways, and a roadmap to further develop GLEAM is presented in Section 7.3.1.

Within the frame of this dissertation, different global data sets of terrestrial evaporation and root-zone soil moisture derived using GLEAM v3 were made available via www.gleam.eu (last visit: 18 November 2019) to foster research and applications in need for accurate information on terrestrial evaporation from continental to global scales. These data sets are updated annually by making use of the latest available forcing to extend the data sets until near present and they are intensively used in different fields (Figure 7.1), as demonstrated by the more than 2200 registered users and the 160 and 308 citations at Web of Science of Martens *et al.* (2017) and the original paper of Miralles *et al.* (2011b), respectively¹.

Data sets from GLEAM are mostly used to study the (global) water cycle and its dynamics: Martens *et al.* (2018b) and Miralles *et al.* (2014) for instance used GLEAM data to investigate the impact of internal climate variability on the dynamics of terrestrial evaporation, a necessary step to properly disentangle the effects of climate change on hydrology (Zhu *et al.*, 2017; Gonsamo *et al.*, 2016; Miralles *et al.*, 2014; Stocker *et al.*, 2013; Trenberth, 2011). Trends in terrestrial evaporation due to our changing climate have also been investigated using GLEAM (e.g. Blunden and Arndt, 2019; Yang *et al.*, 2019; Zhang *et al.*, 2016b; Greve *et al.*, 2014; Miralles *et al.*, 2014), providing critical insights on the impact of climate change on the hydrological cycle and its expected intensification (e.g. Greve *et al.*, 2014).

Data have also been used to aid and optimise water resources management. Keune and Miralles (2019) for instance showed that up to 74% of summer precipitation in European watersheds depends on terrestrial evaporation in

¹Statistics were retrieved at 22 November 2019.

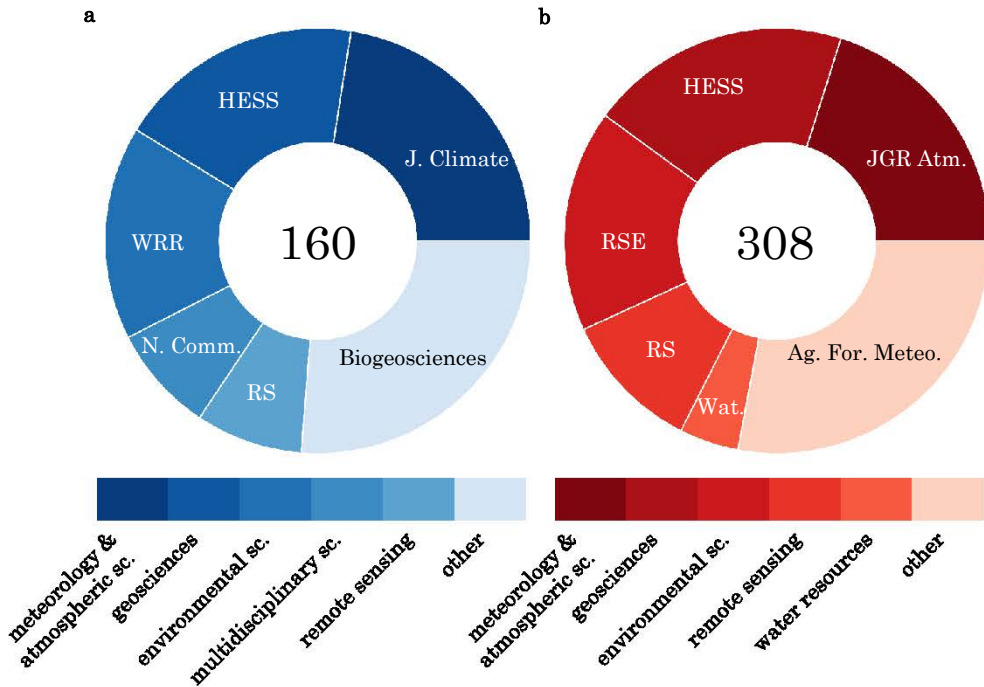


Figure 7.1: Overview of the scientific fields using GLEAM-derived data sets and the total number of citations of (a) Martens *et al.* (2016) and (b) Miralles *et al.* (2011b). Visualisations show the total number of citations in the center of the donut and slices are proportional to the primary scientific field (represented by different colours) in which these scientific articles are published. The journals listed in each slice correspond to the dominant journal using GLEAM-derived data within that scientific field. Journal titles are abbreviated as follows: Journal of Climate (J. Climate), Hydrology and Earth System Sciences (HESS), Water Resources Research (WRR), Nature Communications (N. Comm.), Remote Sensing (RS), Journal of Geophysical Research–Atmospheres (JGR Atm.), Remote Sensing of Environment (RSE), Water (Wat.), and Agricultural and Forest Meteorology (Ag. For. Meteo.). Data were retrieved from Web of Science on 22 November 2019.

remote regions, an important aspect that needs to be considered in water management plans. Orth and Destouni (2018) also used data from GLEAM to analyse the impact of European droughts on both terrestrial evaporation and river discharge, as well as the response time of both fluxes to drought; the latter is paramount to develop early-warning systems in order to secure food and fresh water availability. Finally, Han *et al.* (2017) and Venkatesh *et al.* (2020) investigated how biomass burning in Borneo and forest fires in India affect the hydrological cycle, respectively. Han *et al.* (2017) concluded that due to substantial increases in terrestrial evaporation after large-scale biomass burning, sub-surface water reservoirs get depleted, potentially leading

to shortages in fresh water availability.

Data from GLEAM have also been used to evaluate land surface models (e.g. Albergel *et al.*, 2018; Meier *et al.*, 2018), to benchmark reanalysis data sets (e.g. Martens *et al.*, 2019; Draper *et al.*, 2018; Reichle *et al.*, 2017), to evaluate and construct drought indices (e.g. Marvel *et al.*, 2019; Vicente-Serrano *et al.*, 2018), to assess the accuracy of alternative observation-based evaporation products (e.g. Duveiller *et al.*, 2018; Michel *et al.*, 2016; Miralles *et al.*, 2016; Zhang *et al.*, 2016b), and to bias-correct estimates of terrestrial evaporation in modelling studies (e.g. Schumacher *et al.*, 2019; Wang *et al.*, 2017). These studies have (among others) led to an improved understanding on the impact of land cover and land use changes on surface energy partitioning (Meier *et al.*, 2018; Duveiller *et al.*, 2018), on the impact of human-induced climate change on droughts (Marvel *et al.*, 2019), and on the development of mega heatwaves (Schumacher *et al.*, 2019). GLEAM has also been used in numerous land-atmosphere studies (e.g. Schumacher *et al.*, 2019; Miralles *et al.*, 2019; Guillod *et al.*, 2015; Miralles *et al.*, 2014, 2012), leading to important insights on the occurrence of rainfall (Guillod *et al.*, 2015) and the occurrence of hydro-meteorological extremes (Schumacher *et al.*, 2019; Miralles *et al.*, 2019, 2014, 2012).

Terrestrial evaporation and root-zone soil moisture from GLEAM have also been used in studies not directly focusing on the hydrological cycle, climate, or atmosphere, but that are in need of accurate water balance data: in Bauters *et al.* (2019) for instance, data of terrestrial evaporation from GLEAM were used to assess the water balance in tropical rain forests aiming to study the cycling of nitrogen in these ecosystems, while Romero-Mujalli *et al.* (2018) studied the physico-chemical weathering of carbonate in soils at the global scale and its response to changes in atmospheric CO₂ and temperature. Although not yet studied in detail, it has also been hypothesised by Huang *et al.* (2019) that crop forecasting can strongly benefit from accurate data on evaporative stress. Assimilation of such data sets into crop growth models would strongly reduce their forecasting error. Finally, Enenkel *et al.* (2019) showed that weather-based insurance indices that take into account terrestrial evaporation are better able to describe the impact of drought on crop yields, hence better protecting farmers from these extreme conditions, thereby increasing their productivity (Enenkel *et al.*, 2019).

GLEAM-derived data sets are thus not only used in hydrological studies, but also in ecology, climatology, atmospheric sciences, and soil sciences. In addition, it has been hypothesised that also agricultural planning and water resources management could highly benefit from these data sets (Figure 7.1). Based on these results, it can be concluded that the first objective of this dissertation has been achieved.

7.2.2 GLEAM at high spatial resolution

While Chapters 2 and 3 mainly focused on improving GLEAM with the aim to derive global data sets of terrestrial evaporation and root-zone soil moisture at spatial resolutions suitable for global studies (objective 1, Section 1.2), the potential of GLEAM to be applied at resolutions useful for field-scale applications was assessed in Chapter 4 (objective 2, Section 1.2). In this chapter, a high-resolution pilot data set derived using GLEAM was presented for The Netherlands, Flanders, and the west of Germany, providing estimates of root-zone soil moisture and terrestrial evaporation at 100 m spatial resolution.

The estimates of GLEAM were evaluated against in situ measurements from 39 soil moisture sensors and 5 eddy-covariance towers, compared against temporal and spatial characteristics of alternative products (the coarse-scale GLEAM data set from Chapter 3, LSA-SAF daily evaporation, and a Makkink-based evaporation dataset), and analysed for their response to anomalously dry conditions across the study domain. Despite its original goal to be applied at the global scale and coarse spatial resolution only, the temporal evaluation of the high-resolution estimates from GLEAM against in situ data showed the ability of the model to accurately retrieve the dynamics of both surface soil moisture and terrestrial evaporation with substantially higher spatial detail. However, it should be emphasised here again that validation statistics should be interpreted with care as (1) the number of eddy-covariance sites covering the study domain was relatively low and (2) the soil moisture validation was strongly dominated by the high concentration of soil moisture measurements in the Raam catchment. Albeit the similar temporal statistics against in situ measurements obtained across the range of different products, the fine-resolution data set from GLEAM clearly portrayed the highest spatial detail. Unfortunately, a direct and objective evaluation of the latter was not possible given the low density of in situ measurements covering the study domain. Yet, a comparison of the spatial structures in the data set against land cover and soil texture data revealed realistic patterns that could be explained in a physical manner. In addition, the response of terrestrial evaporation to the summer drought in 2013 over The Netherlands was also deemed realistic, supporting the notion that the model can be applied at higher spatial scales. However, the latter analyses could not be supported by an objective evaluation using the in situ data due to the limited data availability.

Overall, it was shown that GLEAM can produce qualitative and spatially-consistent estimates of root-zone soil moisture and terrestrial evaporation at spatial resolutions useful for agriculture and water management. As the algorithm is designed to rely (to a large extent) on microwave-based data sets of environmental forcing variables, resulting in all-weather output, it has an indisputable advantage over more traditional approaches applied at regional scales based on optical and TIR data. However, given the rather small study

area, its consistently wet climate, and its mild topography, conclusions from this pilot study should be interpreted with care, and the ability of GLEAM to be applied at high resolutions should be further investigated. Therefore, the methodology should be applied for different hydro-climatological regimes – especially water-limited regions and topographically more complex areas – to evaluate the model assumptions. In particular, it is expected that in more complex terrain a detailed description of the lateral movement of water, infiltration, and surface run off – processes that are currently not considered in GLEAM – will become important to properly estimate the root-zone soil moisture and resulting evaporative stress (Section 7.3.1). In addition, due to the high resolution, grid cells might become dominated by specific land cover types and the universal stress function currently implemented in GLEAM might need to be revised to properly model the response of specific land cover types to evaporative stress. Finally, although that the validations did not point towards systematic problems due to the use of the rather coarse atmospheric forcing (as compared to the target resolution), this assumption needs to be further evaluated and alternative forcing needs to be considered in the future.

Altogether, the pilot study presented in Chapter 4 has provided useful insights on the applicability of GLEAM at high resolutions and has fostered the exploration of GLEAM at these resolutions. The latter is evidenced by the ET-Sense project, funded by the BELgian Science Policy Office (BELSPO) in 2018, which aims to derive a high-resolution (1 km) data set of terrestrial evaporation over Europe using GLEAM. Based on the results presented in Chapter 4, it can be concluded that local-scale water management and agricultural planning could potentially benefit substantially from these high-resolution data sets of terrestrial evaporation and that, therefore, the second objective of this dissertation has been achieved.

7.2.3 Showcasing the value of GLEAM

Finally, to demonstrate the assets of the global data sets of terrestrial evaporation from GLEAM (objective 3, Section 1.2), these data sets were used in two relevant applications where (1) the surface energy partitioning in ERA5 was evaluated (Chapter 5) and (2) the impact of internal climate variability on terrestrial evaporation was analysed (Chapter 6). Aside from showing the usefulness of these data sets for global hydrology and model benchmarking, results from these studies also led to a better understanding of the multi-decadal dynamics of terrestrial evaporation and the quality of state-of-the-art reanalysis data.

In summary, results from Chapter 5 showed that the quality of surface energy partitioning in ERA5 is substantially better than in its predecessor ERA-I. However, it was also shown that – based on different analyses with independent reference data – the surface latent heat flux in ERA5 is still

substantially overestimated, although improvements could be seen upon ERA-I. Using GLEAM, it could also be shown that the land surface model implemented in ERA5 could probably benefit from revising the response of terrestrial evaporation to environmental stressors, especially in (semi-)arid regions. However, similar to the analyses in Chapters 2–4, results presented in Chapter 5 should be interpreted while accounting for the limitations of the reference data sets used. Especially the lack of eddy-covariance data in certain regions and the low number of sites available in total, make it difficult to extrapolate conclusions to different areas. In addition, the estimates of the turbulent fluxes based on the water and energy-balance approach (Section 5.2.3) might be – next to errors in the data – compromised by the assumptions that the ground heat flux was a fixed fraction of net radiation and that no changes in water and energy storage occurred within the aggregation period. Although the latter assumption can be justified in natural systems because of the annual temporal resolution used, it may be invalid in densely-populated regions that are prone to substantial human water consumption (Miralles *et al.*, 2016).

In Chapter 6 it was shown – based on an analysis of GLEAM data (among others) – that in about half of the land surface, terrestrial evaporation dynamics are significantly driven by modes of internal climate variability, mainly through their impact on the atmospheric demand for water. It was also shown that ENSO affects dynamics in terrestrial evaporation across the largest part of the global land surface, but that other modes are typically more dominant. It should be emphasised here that the model framework used in Chapter 6 has proven to provide meaningful insights on the impact of internal climate variability on terrestrial evaporation, but that some limitations need to be further addressed in the near future to fully exploit the results. As the results are purely based on an data-driven approach, physically-based modelling might help to better understand the complex interactions between the major modes of climate variability and land surface processes such as terrestrial evaporation. Also the record length has deemed too short to properly investigate the impact of multi-decadal variations caused by for instance AMO. Longer records would also allow to use more complex (highly non-linear) learning methods to better disentangle the effects of internal climate variability, and to properly assess the model fit by defining a separate test set (Section 6.2.2). Despite that the primary objective of the study in Chapter 6 was to detect hot spots of interaction between internal climate variability and terrestrial evaporation, more complex data-driven models – with potentially higher explanatory power – could also increase the usefulness of the method in seasonal forecasting systems.

In conclusion, the studies presented in Chapters 2–4 have resulted in state-of-the-art data sets of terrestrial evaporation and root-zone soil moisture, and important insights on the applicability of GLEAM at high spatial resolutions. With this, the work presented in these chapters has provided important scientific

knowledge and data to partly fill the research gaps defined by Fisher *et al.* (2017). In particular, the data sets derived in this dissertation help to better understand land–atmosphere feedbacks, allow to investigate the impact of variations in climate on global hydrology, and aid managing our water resources in a sustainable way (Section 3.6). The added value of these data sets has also been showcased in the studies presented in Chapters 5 and 6, from which insights on the quality of the surface energy partitioning in ERA5 were obtained and on the impact of internal climate variability on terrestrial evaporation. Altogether, it can be concluded that the objectives defined in Section 1.2 have been achieved.

7.3 Perspectives and challenges

7.3.1 Advancing GLEAM

In 2020, GLEAM will celebrate its tenth anniversary. Ever since its birth in 2010, the model has been progressively improved with the aim to provide better estimates of terrestrial evaporation and root-zone soil moisture to support different scientific disciplines and applications. The data sets are widely used in various scientific fields and the improvements in the model and corresponding data sets have generally been appreciated by their users. With the aspiration to keep on improving the GLEAM data sets, the model can benefit from a wide range of potential algorithmic changes and the incorporation of better – and even new – observational data sets to constrain the model. More specifically, the ten most promising directions² to further develop GLEAM might be to:

1. **Consider interception loss by low vegetation types.** Only forest interception loss is currently simulated in GLEAM. Despite the challenges to measure the volumes intercepted by lower vegetation types, such as shrubs and grasslands, these fluxes might be considerable (Dunkerley, 2000) and important to properly disentangle the total portion of interception loss (Shuttleworth, 2007; Savenije, 2004).
2. **Consider the vertical structure of ecosystems.** The land surface in GLEAM is currently only conceptualised horizontally (i.e. only horizontal variations in land cover are considered), while the vertical structure of the vegetation is not considered (e.g. evaporation from bare soil covered by vegetation is not considered). In spite of relatively low contributions from the understory, or bare soil covered by vegetation, to the total flux of terrestrial evaporation due to the blocking of direct sunlight and lower

²Most of these suggestions might also be applicable to alternative models, ranging from methods aiming at accurately estimating terrestrial evaporation to more complex land surface or climate models.

aerodynamic turbulence (Holwerda and Meesters, 2019; Raz-Yaseef *et al.*, 2010), it is important to model the process, especially in regions with a strong vertical vegetation structure such as tropical forests (Wohl *et al.*, 2012). Such improvements (together with the ones described in Item 1) will also lead to a better partitioning of terrestrial evaporation into its components, a critical task given their different response to the changing climate (Berg and Sheffield, 2019a,b). Note that this partitioning has proven to be poor in existing models (including GLEAM) by studies from e.g. Talsma *et al.* (2018a,b) and Miralles *et al.* (2016).

3. **Improve the modelling of root access to water.** Considering whether the vegetation has access to groundwater or not (e.g. by using information on rooting depth and average groundwater levels), nor variations in groundwater depth are presently considered in GLEAM, but might impact terrestrial evaporation in many regions across the global land surface (Tian *et al.*, 2019a,b; Maxwell and Condon, 2016; Fan *et al.*, 2013; Miguez-Macho and Fan, 2012). In addition, GLEAM does not consider changes in rooting depth, an aspect that might substantially improve the modelled access to water by plants (Fan *et al.*, 2017; Lai and Katul, 2000).
4. **Improve the modelling of evaporation over under-sampled land cover types.** To date, estimates of terrestrial evaporation from GLEAM have been intensively validated across the global domain, mainly using eddy-covariance measurements, and it has been shown that the model tends to perform well across a wide range of hydro-climatic regimes and associated land cover conditions. However, conditions that are commonly less represented in such validation data sets and that have received less attention, are specific land covers like peatlands, snow or ice-covered surfaces, urban areas, and open water (Zhan *et al.*, 2019). Although specific parameterisations of the Priestley and Taylor equation are already used in GLEAM for some of these land cover types (Murphy and Koop, 2005), the former has never been intentionally designed for this purpose (Priestley and Taylor, 1972), nor has its use in GLEAM for these specific conditions ever been validated.
5. **Revise the model assumptions aiming at the high-resolution application of GLEAM.** Assumptions that have been made upon the development of GLEAM that specifically relate to the coarse spatial resolution will need to be revised, and other physical processes – such as sub-surface lateral flow and overland flow – might need to be implemented to make the model valid at high spatial resolutions.

6. **Model the diurnal cycle of terrestrial evaporation.** Water resources management would greatly benefit from sub-daily estimates of terrestrial evaporation (Sheffield *et al.*, 2018). Trying to estimate the diurnal cycle of terrestrial evaporation has already been briefly explored by GLEAM (Chapter 2). However, properly modelling this cycle requires the re-formulation of several components currently implemented in GLEAM, such as the interception loss model that was originally designed for daily resolutions (Miralles *et al.*, 2010), the proper consideration of night-time evaporation which might be an important fraction of the total daily flux (Padrón *et al.*, 2019), and a proper modelling of soil conductivity (and its dynamics) in the simple water-balance model.
7. **Consider the stomatal response to CO₂ fertilisation.** It has been shown that under rising atmospheric CO₂ concentrations, plants become more efficient in assimilating carbon and thus decrease their stomatal conductance; i.e. less water is lost via transpiration for the same amount of carbon fixated in plant tissues (e.g. Berg and Sheffield, 2019a; Ukkola *et al.*, 2015). The latter is also known as water-use efficiency and is currently not considered in GLEAM, an issue that mainly hampers the use of GLEAM-derived data sets for the analysis of trends in terrestrial evaporation due to climate change. Considering water-use efficiency in GLEAM would require the use of alternative (physically-based) equations to estimate potential evaporation and, especially, evaporative stress.
8. **Model the two-way response of terrestrial evaporation to VPD.** Currently, the response of terrestrial evaporation to changes in VPD is not explicitly modelled in GLEAM. While higher values of VPD typically result in higher potential evaporation rates, at the same time, they increase the stomatal resistance of plants, and thus result in higher evaporative stress (Konings and Gentine, 2017). However, high VPD typically occurs along with low soil moisture and the effect of soil moisture and VPD on the reduced stomatal conductance is still under investigation (Konings and Gentine, 2017). Nevertheless, properly modelling this effect is important to accurately capture evaporative stress, especially in anomalously dry conditions, which are projected to occur more often as a result of global warming.
9. **Explore the assets of new observational data sets.** GLEAM can strongly benefit from the ever-growing stack of satellite-based geophysical variables (McCabe *et al.*, 2017a) and the increasing spatio-temporal resolution of the available data from e.g. drones and cubesats (e.g. Houborg and McCabe, 2018; Manfreda *et al.*, 2018; McCabe *et al.*, 2017b; Hoffmann *et al.*, 2016; Sobrino *et al.*, 2016). A promising way forward is the use of data sets related to vegetation stress to better constrain the

estimates of potential evaporation such as LST (Sobrino *et al.*, 2016) or Solar-Induced Fluorescence (SIF), which has already been shown to be a proxy of environmental stress on transpiration (Pagán *et al.*, 2019). Variations in groundwater derived from the Gravity Recovery And Climate Experiment (GRACE) satellite might also prove valuable to incorporate groundwater level dynamics in GLEAM (Item 3).

10. **Implement innovative data assimilation techniques to deal with the plethora of observational data to constrain GLEAM.** The plethora of useful data sets to better constrain GLEAM also presents great challenges on how to properly incorporate this information into the model. While some of these data sets can be used to force GLEAM, others need to be ingested in an alternative way. Advanced data assimilation techniques capable of dealing with these huge volumes of biased data are an encouraging means to achieve this goal. In this respect, proper observation operators need to be implemented in GLEAM and much can be learned from operational weather forecast centers such as ECMWF where different observation-based data sets have already been assimilated in atmospheric models for many years (Dee *et al.*, 2011; Shuttleworth, 2007).

7.3.2 Challenges in evaporation science

Despite big steps that have been taken in the last decade in the field of evaporation science, terrestrial evaporation is still one of the most uncertain components of the global hydrological cycle (Fisher *et al.*, 2017; McCabe *et al.*, 2017a; Harrigan and Berghuijs, 2016; Dolman *et al.*, 2014; Dolman and de Jeu, 2010). Over the last years, research has mainly focused on the development and refinement of algorithms to derive terrestrial evaporation from satellite observations, strongly driven by international activities such as NASA's NEWS study, the European Union WATCH project, the GEWEX LandFlux initiative, and ESA's WACMOS project. Such studies have resulted in the proliferation of data sets with unique spatio-temporal detail, coverage in time and space, and skill in estimating terrestrial evaporation (Gomis-Cebolla *et al.*, 2019; Talsma *et al.*, 2018a; McCabe *et al.*, 2016; Michel *et al.*, 2016; Miralles *et al.*, 2016; Mueller *et al.*, 2013; Jiménez *et al.*, 2011). Their differences present an opportunity to merge them into a superior product, which might be the way forward to attain the accuracy and spatio-temporal detail necessary to advance the field (Clayson *et al.*, 2019; Stoy *et al.*, 2019; Sheffield *et al.*, 2018). Several studies have already explored the merging of different resources of terrestrial evaporation, ranging from simple averaging (e.g. Jiménez *et al.*, 2018; Mueller *et al.*, 2013) to more advanced techniques where products are combined in an apparent optimal way based on their relative uncertainties (e.g. Hobeichi

et al., 2018; Jiménez *et al.*, 2018; Yao *et al.*, 2017; Martens *et al.*, 2018b; Aires, 2014; Jung *et al.*, 2011), a challenging task at the global scale given the rather low density of in situ measurement networks for error characterisation and the correlated nature of these errors (Jiménez *et al.*, 2018; Khan *et al.*, 2018; Aires, 2014). Others have directly fused in situ measurements with satellite-based geophysical variables to derive global estimates of terrestrial evaporation with machine learning algorithms (e.g. Jung *et al.*, 2019, 2011, 2010, 2009). Except for the objective characterisation of errors, other grand challenges in the merging of data sets become increasingly important with the growth of available data. Most studies so far have for instance only focused on merging data sets with similar spatio-temporal properties, but much can be gained by exploring the merging of fine and coarse resolution data (either in space or time), a challenging but interesting path for future research.

Next to model development, further investing in Earth observation programs – such as the Sentinel missions within the Copernicus program (Figure 1.1b) from ESA³ – to monitor different geophysical variables related to terrestrial evaporation and developing dedicated space missions to study the flux – such as ECOSTRESS (Hulley *et al.*, 2017) – are promising means to further advance the field of evaporation science (Sheffield *et al.*, 2018; Tauro *et al.*, 2018; Fisher *et al.*, 2017; Hulley *et al.*, 2017; McCabe *et al.*, 2017a). Existing algorithms to derive terrestrial evaporation from satellite data are currently being optimised to run at finer spatial resolutions (e.g. Martens *et al.*, 2018a; McCabe *et al.*, 2017b), but their full deployment at relevant scales is mainly hampered by the spatial resolution of the existing stack of observation-based forcing they rely on (McCabe *et al.*, 2017a). Innovative sensors on cubesats and drones already provide useful data for evaporation monitoring in the visible and near-infrared spectrum at unprecedented spatial resolution (Houborg and McCabe, 2018; Manfreda *et al.*, 2018; McCabe *et al.*, 2017b; Hoffmann *et al.*, 2016); however observations at longer wavelengths, such as in the microwave domain, that are less sensitive to clouds are to date not yet available at the same spatial resolution. Also in situ networks should be maintained and, preferentially intensified, to enable the global-scale validation of terrestrial evaporation and to meet the growing demands for in situ validation data (Sheffield *et al.*, 2018). In addition, in situ networks should be better distributed across the globe, efforts should be made to sample areas that are particularly sensitive to our changing climate such as high northern latitudes and Africa – currently being under-sampled (Clayson *et al.*, 2019; Baldocchi *et al.*, 2001) – and more focus

³Currently, six mission concepts that should fill gaps in the Copernicus user needs and extent the capabilities of the existing Copernicus program are being studied. Some of these missions will provide important information for the evaporation community such as LST, land cover data, atmospheric CO₂ concentration, and soil moisture. More information can be found at http://www.esa.int/Applications/Observing_the_Earth/Copernicus/Copernicus_High_Priority_Candidates; last visit: 18 November 2019.

should be directed towards measuring the separate components of terrestrial evaporation in the field (Stoy *et al.*, 2019; Talsma *et al.*, 2018a). Ultimately, in situ measurement techniques, networks, and validation tools should be re-designed to cope with the increasing spatial resolution of regional and continental data sets and to allow the validation of their spatial and temporal details (Martens *et al.*, 2018a). In this sense, the deployment of core validation sites for terrestrial evaporation, analogous to core soil moisture validation networks, could be a promising path forward.

In addition to further advancing algorithms and in situ measurement networks, priority should also be given to make data accessible not only to scientists, but also to operational centres, water authorities, and agricultural institutes in order to exploit the full potential of the existing data. Given the importance of information on terrestrial evaporation for monitoring and forecasting hydro-meteorological events such as floods and droughts, water resources management in general, and agricultural planning (Otkin *et al.*, 2016; Sheffield *et al.*, 2012), a community-effort should thus be made to make data available in near-real time and free of charge, whenever possible (Sheffield *et al.*, 2018).

Finally, studying the impacts of our changing climate – arguably one of the most important challenges of our generation – on our biosphere and its processes will be of key importance to mitigate and adapt to these changes. Given the importance of terrestrial evaporation in the climate system, analysing the impact of changes on the flux can thus provide valuable insights. Climatic studies might benefit from observation-based data sets of terrestrial evaporation in two ways as (1) the reliability of climate projections depends on the accuracy of climate model simulations; observational benchmarks are thus a necessary means to properly analyse the quality of these simulations (e.g. Berg and Sheffield, 2019a,b), and (2) the analysis of historical records provides useful insights for the future (e.g. Forzieri *et al.*, 2019; Martens *et al.*, 2018a; Miralles *et al.*, 2014; Jung *et al.*, 2010). Unfortunately, observational records of terrestrial evaporation (and any other geophysical variable) based on satellite data only span the last four decades at most. While reanalyses might nowadays provide longer records starting half way the twentieth century (Hersbach *et al.*, 2018), they are less constrained by observations and more tight to model physics than satellite-based retrievals. In addition, their coverage is still too short for evaluating the temporal dynamics of geophysical variables over multi-decadal scales; especially when the variable under consideration is affected by low-frequency variations (i.e. with a period close to – or larger than – the observational record) induced by for instance internal modes of climate variability such as AMO. In this respect, records of tree-ring indices, which can be used as a proxy for vegetation activity and are basically a fingerprint of variations in many environmental variables (St. George, 2014), might

provide valuable and complementary information to existing satellite records of different variables of interest, including terrestrial evaporation, soil moisture, precipitation, air temperature, drought indices, and vegetation greenness (e.g. Marvel *et al.*, 2019; Tronquo, 2019; Babst *et al.*, 2018; Mergaert, 2018; Baek *et al.*, 2017; Coulthard *et al.*, 2017; Babst *et al.*, 2017; Vicente-Serrano *et al.*, 2016; Rammig *et al.*, 2015; de Jeu *et al.*, 2012). Although sampling locations for trees have historically been optimised for paleo-climatological studies (Babst *et al.*, 2018), the expansion and maintenance of existing networks – and fusing their observations with satellite-based records – might strongly boost the Earth-system science community in their quest for answers that nowadays cannot be given due to the limited record length of satellite-based observations (Babst *et al.*, 2017).

Eddy-covariance data

Table A.1: List of the OzFlux sites used in Chapter 2 together with their FLUXNET code (ID), IGBP land cover (LC), official reference, the Pearson correlation coefficient for the GLEAM OL against the in situ data (R_{OL}), and the Pearson correlation coefficient for the experiment where the combined ascending-descending SMOS data set is assimilated into GLEAM using a constant quality factor against the in situ data (R_{DA}).

ID	LC	Reference	R_{OL} (-)	R_{DA} (-)
AU-ASM	ENF	Cleverly (2011)	0.79	0.71
AU-Cpr	SAV	Calperum Tech (2013)	0.81	0.82
AU-DaS	SAV	Beringer (2013b)	0.83	0.85
AU-Dry	SAV	Beringer (2013c)	0.80	0.80
AU-Emr	GRA	Schroder (2014)	0.70	0.70
AU-GWW	SAV	Macfarlane (2013)	0.82	0.81
AU-RDF	WSA	Beringer (2014a)	0.65	0.71
AU-Rig	GRA	Beringer (2014b)	0.66	0.66
AU-Stp	GRA	Beringer (2013d)	0.81	0.81
AU-TTE	OSH	Cleverly (2013a)	0.71	0.70
AU-Whr	WSA	Cleverly (2013b)	0.77	0.79
AU-Ync	GRA	Beringer (2013e)	0.66	0.62

Table A.2: List of the FLUXNET sites used in Chapter 3 together with their FLUXNET code (ID), IGBP land cover (LC), official reference (or principal investigator (PI)), and the Pearson correlation coefficient for the GLEAM v3.0a ($R_{v3.0a}$), v3.0b ($R_{v3.0b}$), and v3.0c ($R_{v3.0c}$) data sets against the in situ data.

ID	LC	Reference/PI	$R_{v3.0a}$	$R_{v3.0b}$	$R_{v3.0c}$
AT-Neu	GRA	George Wohlfahrt	0.89	0.89	–
AU-ASM	ENF	Cleverly (2011)	0.90	0.88	0.85
AU-Cpr	SAV	Calperum Tech (2013)	0.67	0.66	0.70
AU-DaP	GRA	Beringer (2013a)	0.92	0.93	0.94
AU-DaS	SAV	Beringer (2013b)	0.84	0.85	0.85
AU-Dry	SAV	Beringer (2013c)	0.88	0.86	0.84
AU-Emr	GRA	Schroder (2014)	0.61	0.60	0.57
AU-GWW	SAV	Macfarlane (2013)	0.72	0.65	0.66
AU-RDF	WSA	Beringer (2014a)	0.60	0.61	0.58
AU-Rig	GRA	Beringer (2014b)	0.41	0.31	0.32
AU-Stp	GRA	Beringer (2013d)	0.91	0.89	0.89
AU-TTE	OSH	Cleverly (2013a)	0.88	0.88	0.86
AU-Ync	GRA	Beringer (2013e)	0.67	0.61	0.62
BE-Bra	MF	Carrara <i>et al.</i> (2004)	0.84	–	–
BE-Lon	CRO	Moureaux <i>et al.</i> (2006)	0.76	–	–
BE-Vie	MF	Aubinet <i>et al.</i> (2001)	0.86	–	–
BR-Sa3	EBF	Steininger (2004)	0.28	–	–
CA-Gro	MF	McCaughey <i>et al.</i> (2006)	0.84	0.85	–
CA-NS7	OSH	Bond-Lamberty <i>et al.</i> (2004)	0.85	–	–
CA-Obs	ENF	Bond-Lamberty <i>et al.</i> (2004)	0.86	–	–
CH-Cha	GRA	Shijie Han	0.91	0.91	0.90
CH-Dav	ENF	Lukas Hoertnagl	0.71	0.70	0.74
CH-Fru	GRA	Zeeman <i>et al.</i> (2010)	0.87	0.88	0.88
CH-Oe1	GRA	Christof Ammann	0.93	0.93	–
CH-Oe2	CRO	Christof Ammann	0.86	0.86	–
CN-Cha	MF	Shijie Han	0.91	0.87	–
CN-Cng	GRA	Gang Dong	0.88	0.90	–
CN-Dan	GRA	Shi Peili	0.85	–	–
CN-Din	EBF	Guoyi Zhou	0.72	0.78	–
CN-Du2	GRA	Chen Shiping	0.87	0.89	–
CN-Ha2	WET	Yingnian Li	0.95	–	–
CN-HaM	GRA	Kato <i>et al.</i> (2006)	0.91	–	–
CN-Qia	ENF	Huimin Wang	0.86	0.85	–
CZ-BK1	ENF	Marian Pavelka	0.80	0.83	0.86
CZ-BK2	GRA	Marian Pavelka	0.87	0.89	0.87
CZ-wet	WET	Marian Pavelka	0.92	0.93	0.94
DE-Geb	CRO	Antje Moffat	0.84	–	–
DE-Gri	GRA	Christian Bernhofer	0.89	–	–
DE-Hai	DBF	Knohl <i>et al.</i> (2003)	0.89	–	–
DE-Kli	CRO	Christian Bernhofer	0.82	–	–
DE-Lkb	ENF	Rainer Steinbrecher	0.78	0.80	–
DE-Lnf	DBF	Alexander Knohl	0.89	–	–
DE-Obe	ENF	Christian Bernhofer	0.84	–	–
DE-RuR	GRA	Borchard <i>et al.</i> (2015)	0.91	–	–
DE-Seh	CRO	Karl Schneider	0.76	–	–
DE-Tha	ENF	Christian Bernhofer	0.86	–	–
FI-Hyy	ENF	Timo Vesala	0.88	–	–
FI-Sod	ENF	Tuomas Laurila	0.87	–	–
FR-Fon	DBF	Bazot <i>et al.</i> (2013)	0.85	0.86	0.84
FR-Gri	CRO	Pierre Cellier	0.75	0.76	–
IT-Col	DBF	Giorgio Matteucci	0.68	0.66	0.61
IT-La2	ENF	Alessandro Cescatti	0.83	–	–
IT-Lav	ENF	Damiano Gianelle	0.78	0.77	0.81

Table A.2: Eddy-covariance data used in Chapter 3 (continued).

ID	LC	Reference/PI	$R_{v3.0a}$	$R_{v3.0b}$	$R_{v3.0c}$
IT-MBo	GRA	Damiano Gianelle	0.85	0.89	–
IT-PT1	DBF	Günther Seufert	0.86	–	–
IT-Ren	ENF	Stefano Minerbi	0.76	0.82	0.84
IT-Tor	GRA	Galvagno <i>et al.</i> (2013)	0.91	–	–
RU-Fyo	ENF	Milyukova <i>et al.</i> (2002)	0.78	–	–
SD-Dem	SAV	Ardö <i>et al.</i> (2008)	0.93	0.93	–
US-AR1	GRA	David Billesbach	0.82	0.85	0.72
US-AR2	GRA	David Billesbach	0.77	0.76	–
US-ARM	CRO	Fischer <i>et al.</i> (2007)	0.71	0.72	0.70
US-ARb	GRA	Margaret Torn	0.80	0.81	–
US-ARc	GRA	Margaret Torn	0.82	0.83	–
US-Blo	ENF	Goldstein <i>et al.</i> (2000)	0.73	0.60	–
US-Cop	GRA	David Bowling	0.51	–	–
US-GLE	ENF	Arain and Restrepo-Coupe (2005)	0.38	0.34	0.38
US-Goo	GRA	Tilden Meyers	0.88	0.90	–
US-Ha1	DBF	Goulden <i>et al.</i> (1996)	0.80	0.84	0.88
US-Ivo	WET	McEwing <i>et al.</i> (2015)	0.82	–	–
US-LWW	GRA	Twine <i>et al.</i> (2000)	0.89	–	–
US-MMS	DBF	Schmid <i>et al.</i> (2000)	0.89	0.90	0.89
US-Me2	ENF	Campbell and Law (2005)	0.75	0.76	0.79
US-Me3	ENF	Bond-Lamberty <i>et al.</i> (2004)	0.88	0.86	–
US-Me5	ENF	Irvine <i>et al.</i> (2004)	0.71	–	–
US-Me6	ENF	Ruehr <i>et al.</i> (2012)	0.85	0.86	0.86
US-NR1	ENF	Arain and Restrepo-Coupe (2005)	0.73	0.56	0.56
US-Ne1	CRO	Simbahan <i>et al.</i> (2006)	0.76	0.81	0.75
US-Ne2	CRO	Amos <i>et al.</i> (2005)	0.76	0.80	0.80
US-Ne3	CRO	Verma <i>et al.</i> (2005)	0.77	0.81	0.77
US-Oho	DBF	Noormets <i>et al.</i> (2008)	0.80	0.82	0.87
US-PFa	MF	Richardson <i>et al.</i> (2006)	0.83	0.85	0.84
US-SRC	OSH	Shirley Kurc	0.80	0.78	0.65
US-SRG	GRA	Biederman <i>et al.</i> (2016)	0.84	0.85	0.83
US-SRM	WSA	Scott <i>et al.</i> (2009)	0.79	0.81	0.80
US-Ton	WSA	Chen <i>et al.</i> (2007)	0.89	0.87	0.88
US-Var	GRA	Ma <i>et al.</i> (2007)	0.74	0.72	0.74
US-WCr	DBF	Cook <i>et al.</i> (2004)	0.80	0.85	0.84
US-Whs	OSH	Scott (2010)	0.85	0.84	0.89
US-Wkg	GRA	Scott <i>et al.</i> (2010)	0.80	0.81	0.88
ZA-Kru	SAV	Bob Scholes	0.81	0.78	–

Table A.3: List of the FLUXNET sites used in Chapter 4 together with their FLUXNET code (ID), IGBP land cover (LC) and official reference (or principal investigator (PI)).

ID	LC	Reference/PI
BE-Bra	MF	Carrara <i>et al.</i> (2004)
DE-RuR	GRA	Borchard <i>et al.</i> (2015)
DE-RuS	CRO	Eder <i>et al.</i> (2015)
NI-Ca1	GRA	Chen <i>et al.</i> (1997)
NI-Loo	ENF	Eddy Moors

Table A.4: List of the FLUXNET sites used in Chapter 5 together with their FLUXNET code (ID), IGBP land cover (LC) and official reference (or principal investigator (PI)).

ID	LC	Reference/PI	ID	LC	Reference/PI
AR-Slu	MF	Gabriela Posse	FI-Sod	ENF	Tuomas Laurila
AT-Neu	GRA	George Wohlfahrt	FR-Fon	DBF	Bazot <i>et al.</i> (2013)
AU-ASM	ENF	Cleverly (2011)	FR-Gri	CRO	Pierre Cellier
AU-Cpr	SAV	Calperum Tech (2013)	FR-LBr	ENF	Denis Loustau
AU-Cum	EBF	Elise Pendall	FR-Pue	EBF	Richard Joffre
AU-DaP	GRA	Beringer (2013a)	IT-CA1	DBF	Dario Papale
AU-DaS	SAV	Beringer (2013b)	IT-CA2	CRO	Beniamino Gioli
AU-Dry	SAV	Beringer (2013c)	IT-CA3	DBF	Dario Papale
AU-Emr	GRA	Schroder (2014)	IT-Col	DBF	Giorgio Matteucci
AU-GWW	SAV	Macfarlane (2013)	IT-Isp	DBF	Ferréa <i>et al.</i> (2012)
AU-Gin	WSA	Richard Silberstein	IT-La2	ENF	Alessandro Cescatti
AU-RDF	WSA	Beringer (2014a)	IT-Lav	ENF	Damiano Gianelle
AU-Rig	GRA	Beringer (2014b)	IT-MBo	GRA	Damiano Gianelle
AU-Stp	GRA	Beringer (2013d)	IT-PT1	DBF	Günther Seufert
AU-TTE	OSH	Cleverly (2013a)	IT-Ren	ENF	Stefano Minerbi
AU-Tum	EBF	Eva Van Gorsel	IT-Ro1	DBF	Dario Papale
AU-Wom	EBF	Stefan Arndt	IT-Ro2	DBF	Dario Papale
AU-Ync	GRA	Beringer (2013e)	IT-Tor	GRA	Galvagno <i>et al.</i> (2013)
BE-Bra	MF	Carrara <i>et al.</i> (2004)	JP-SMF	MF	Takeshi Ohta
BE-Lon	CRO	Moureaux <i>et al.</i> (2006)	MY-PSO	EBF	Satoru Takanashi
BE-Vie	MF	Aubinet <i>et al.</i> (2001)	NL-Loo	ENF	Eddy Moors
BR-Sa3	EBF	Steininger (2004)	RU-Che	WET	Lutz Merbold
CA-Gro	MF	McCaughey <i>et al.</i> (2006)	RU-Cok	OSH	Han Dolman
CA-Man	ENF	Hirsch <i>et al.</i> (2004)	RU-Fyo	ENF	Milyukova <i>et al.</i> (2002)
CA-NS1	ENF	Goulden <i>et al.</i> (2006)	RU-Ha1	GRA	Dario Papale
CA-NS2	ENF	Hirsch <i>et al.</i> (2004)	SD-Dem	SAV	Ardö <i>et al.</i> (2008)
CA-NS3	ENF	Hirsch <i>et al.</i> (2004)	SE-St1	WET	Thomas Friborg
CA-NS4	ENF	Hirsch <i>et al.</i> (2004)	US-AR1	GRA	David Billesbach
CA-NS5	ENF	Hirsch <i>et al.</i> (2004)	US-AR2	GRA	David Billesbach
CA-NS6	OSH	Hirsch <i>et al.</i> (2004)	US-ARM	CRO	Fischer <i>et al.</i> (2007)
CA-NS7	OSH	Bond-Lamberty <i>et al.</i> (2004)	US-ARb	GRA	Margaret Torn
CA-Oas	DBF	Barr <i>et al.</i> (2002)	US-ARc	GRA	Margaret Torn
CA-Obs	ENF	Bond-Lamberty <i>et al.</i> (2004)	US-Atq	WET	Kwon <i>et al.</i> (2006)
CA-Qfo	ENF	Bergeron <i>et al.</i> (2007)	US-Blo	ENF	Goldstein <i>et al.</i> (2000)
CA-SF1	ENF	Amiro (2009)	US-CRT	CRO	Chu <i>et al.</i> (2014)
CA-SF2	ENF	Amiro (2009)	US-Cop	GRA	David Bowling
CA-TP1	ENF	Arain and Restrepo-Coupe (2005)	US-GLE	ENF	Arain and Restrepo-Coupe (2005)
CA-TPD	DBF	Arain and Restrepo-Coupe (2005)	US-Goo	GRA	Tilden Meyers
CH-Cha	GRA	Shijie Han	US-Ha1	DBF	Goulden <i>et al.</i> (1996)
CH-Dav	ENF	Lukas Hoertnagl	US-IB2	GRA	Roser Matamala
CH-Fru	GRA	Zeeman <i>et al.</i> (2010)	US-Ivo	WET	McEwing <i>et al.</i> (2015)
CH-Oe1	GRA	Christof Ammann	US-KS2	CSH	Hungate <i>et al.</i> (2002)
CH-Oe2	CRO	Christof Ammann	US-LWW	GRA	Twine <i>et al.</i> (2000)
CN-Cha	MF	Shijie Han	US-Los	WET	Denning <i>et al.</i> (2003)
CN-Cng	GRA	Gang Dong	US-MMS	DBF	Schmid <i>et al.</i> (2000)
CN-Dan	GRA	Shi Peili	US-Me2	ENF	Campbell and Law (2005)
CN-Din	EBF	Guoyi Zhou	US-Me3	ENF	Bond-Lamberty <i>et al.</i> (2004)
CN-Du2	GRA	Chen Shiping	US-Me5	ENF	Irvine <i>et al.</i> (2004)
CN-Ha2	WET	Yingnian Li	US-Me6	ENF	Ruehr <i>et al.</i> (2012)
CN-HaM	GRA	Kato <i>et al.</i> (2006)	US-Myb	WET	Dennis Baldocchi
CN-Qia	ENF	Huimin Wang	US-NR1	ENF	Arain and Restrepo-Coupe (2005)
CN-Sw2	GRA	Changliang Shao	US-Ne1	CRO	Simbahan <i>et al.</i> (2006)
CZ-BK1	ENF	Marian Pavelka	US-Ne2	CRO	Amos <i>et al.</i> (2005)
CZ-BK2	GRA	Marian Pavelka	US-Ne3	CRO	Verma <i>et al.</i> (2005)
CZ-wet	WET	Marian Pavelka	US-PFa	MF	Richardson <i>et al.</i> (2006)
DE-Geb	CRO	Antje Moffat	US-SRC	OSH	Shirley Kurc
DE-Gri	GRA	Christian Bernhofer	US-SRG	GRA	Biederman <i>et al.</i> (2016)
DE-Hai	DBF	Knohl <i>et al.</i> (2003)	US-SRM	WSA	Scott <i>et al.</i> (2009)
DE-Kli	CRO	Christian Bernhofer	US-Syv	MF	Desai (2010)
DE-Lkb	ENF	Rainer Steinbrecher	US-Ton	WSA	Chen <i>et al.</i> (2007)
DE-Lnf	DBF	Alexander Knohl	US-Twt	CRO	Hatala <i>et al.</i> (2012)
DE-Obe	ENF	Christian Bernhofer	US-UMB	DBF	Jarvis <i>et al.</i> (2004)
DE-RuR	GRA	Borchard <i>et al.</i> (2015)	US-Var	GRA	Ma <i>et al.</i> (2007)
DE-RuS	CRO	Eder <i>et al.</i> (2015)	US-WCr	DBF	Cook <i>et al.</i> (2004)

Table A.4: Eddy-covariance data used in Chapter 5 (continued).

ID	LC	Reference/PI	ID	LC	Reference/PI
DE-Seh	CRO	Karl Schneider	US-WPT	WET	Chu <i>et al.</i> (2014)
DE-Tha	ENF	Christian Bernhofer	US-Whs	OSH	Scott (2010)
DK-NuF	WET	Thomas Friborg	US-Wi4	ENF	Noormets <i>et al.</i> (2008)
DK-Sor	DBF	Andreas Ibrom	US-Wi9	ENF	Noormets <i>et al.</i> (2008)
ES-LgS	OSH	Andrew Kowalsky	US-Wkg	GRA	Scott <i>et al.</i> (2010)
FI-Hyy	ENF	Timo Vesala	ZA-Kru	SAV	Bob Scholes
FI-Let	ENF	Tuomas Laurila	ZA-Mon	DBF	Werner Kutsch
FI-Lom	WET	Tuomas Laurila			

Bias-correction of radiation components

The fine-scale surface radiation components, i.e. shortwave incoming radiation, reflected shortwave radiation, longwave incoming radiation, and emitted longwave radiation – estimated from several inconsistent data sources (Table 4.1) – are individually scaled towards coarse-scale measurements from CERES (Wielicki, 1996) to obtain consistent fluxes. The scaling involves a multiplicative bias correction of the fine-scale fluxes towards CERES, preserving the spatial detail, but removing the absolute mismatch between the two at the coarse scale.

First, the coarse-scale field (c) is interpolated over the fine-scale grid using a nearest neighbour interpolation. For each pixel i, j in the fine-scale field f , a multiplicative bias correction factor is then calculated by convolving ($*$) the ratio of the fine- and coarse-scale field, with a Gaussian kernel of one-sided width n (Ω^n). The bias-corrected fine-scale value for grid cell i, j can then be calculated as:

$$f_{i,j}^* = f_{i,j} \left[\left(\frac{c}{f} \right) * \Omega^n \right]_{i,j} \quad (\text{B.1})$$

Equation B.1 can also be written as:

$$f_{i,j}^* = f_{i,j} \sum_{p=-n}^n \sum_{q=-n}^n \frac{c_{i+p,j+q}}{f_{i+p,j+q}} \Omega^{p+w+1,q+w+1} \quad (\text{B.2})$$

Equation B.2 shows that the bias-correction factor for pixel i, j in the fine-scale grid is essentially a weighted average of the multiplicative correction factors within a neighbourhood of that pixel. The actual size of the neighbourhood n equals ± 50 km, approximately half of the resolution of CERES. Weights

within the neighbourhood vary according to a Gaussian function with standard deviation equal to one fourth of n , meaning that weights drop rapidly with the distance from pixel i, j , and approach essentially zero for distances >25 km from i, j .

Supplementary figures

C.1 Supplementary figures for Chapter 4

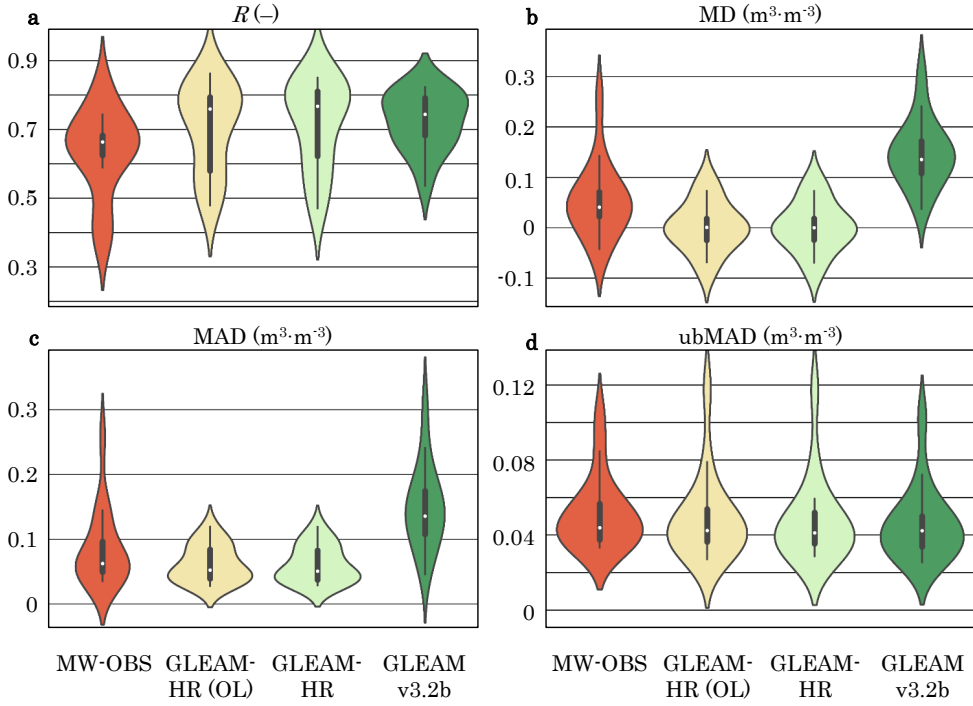


Figure C.1: Violin plots of the validation statistics of surface soil moisture from microwave observations (MW-OBS), GLEAM-HR without data assimilation (OL), GLEAM-HR, and GLEAM v3.2b. **(a)** Violin plots for the Pearson correlation coefficient (R), **(b)** Mean Difference (MD, in situ as a reference), **(c)** Mean Absolute Difference (MAD), and **(d)** unbiased MAD (ubMAD). Individual statistics are calculated for 17 soil moisture sensors located in The Netherlands and violin plots represent the distribution of the statistics with indication of the median (white dot), interquartile range (thick line), and 95% interval (thin line).

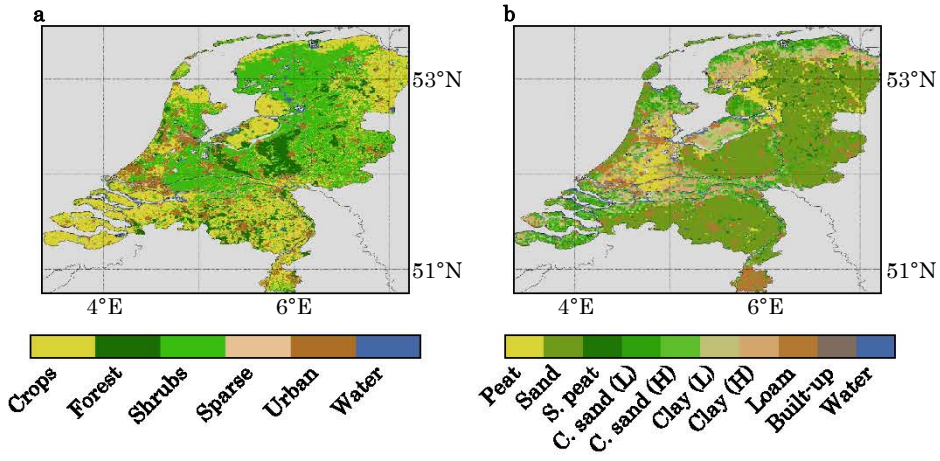


Figure C.2: (a) Land cover obtained from the global ESA CCI land cover classification map (2015), and (b) simplified soil map from WUR - Alterra of The Netherlands (WUR-Alterra, 2006). In (b) “S.”, “C.”, “L”, and “H” refer to “Sandy”, “Clayey”, “Light”, and “Heavy”, respectively.

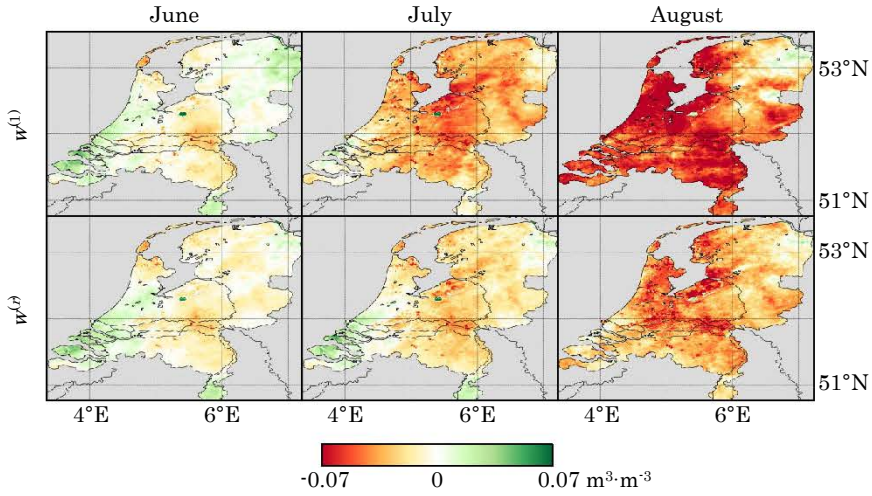


Figure C.3: Maps of the monthly anomalies (relative to the 2013–2017 monthly mean) of surface soil moisture ($w^{(1)}$) and root-zone soil moisture ($w^{(r)}$) from GLEAM-HR for June–August 2013 in The Netherlands.

C.2 Supplementary figures for Chapter 5

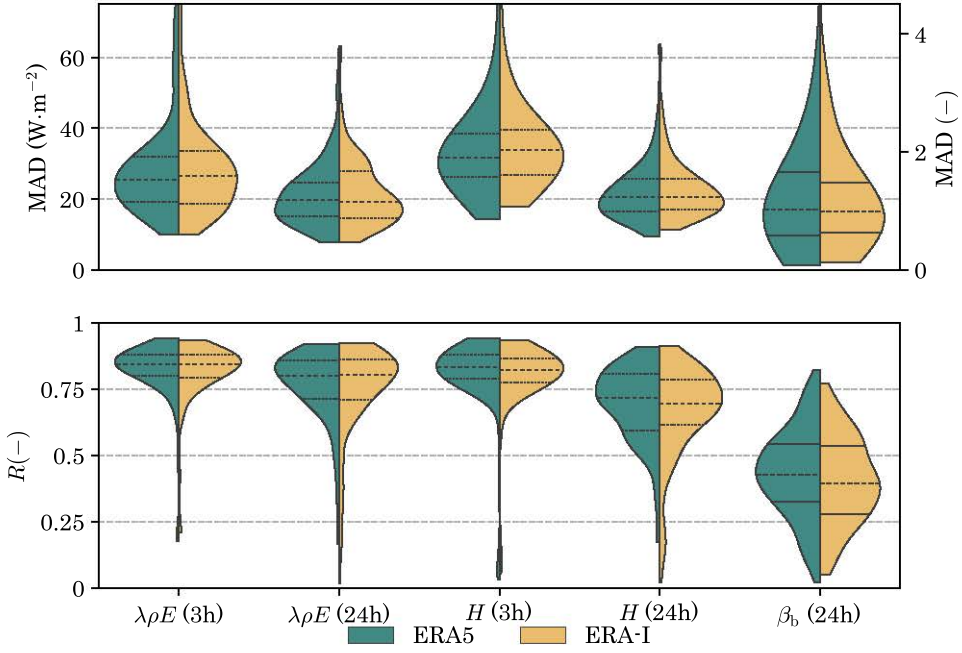


Figure C.4: Violin plots of temporal validation statistics of the surface latent heat flux ($\lambda\rho E$), surface sensible heat flux (H), and Bowen ratio (β_b) from ERA5 (green) and ERA-I (yellow). Statistics are calculated against in situ eddy-covariance measurements at both 3-hourly and daily temporal resolutions. Violin plots represent the distribution of the individual validation statistics with indication of the median and inter-quartile range and are calculated using a kernel density estimation approach. Statistics include the Mean Absolute Difference (MAD, raw in situ time series from 143 sites as reference) and the Pearson correlation coefficient (R , raw in situ time series from 143 sites as reference). For MAD, the distribution of β_b is plotted on the right y-axis.

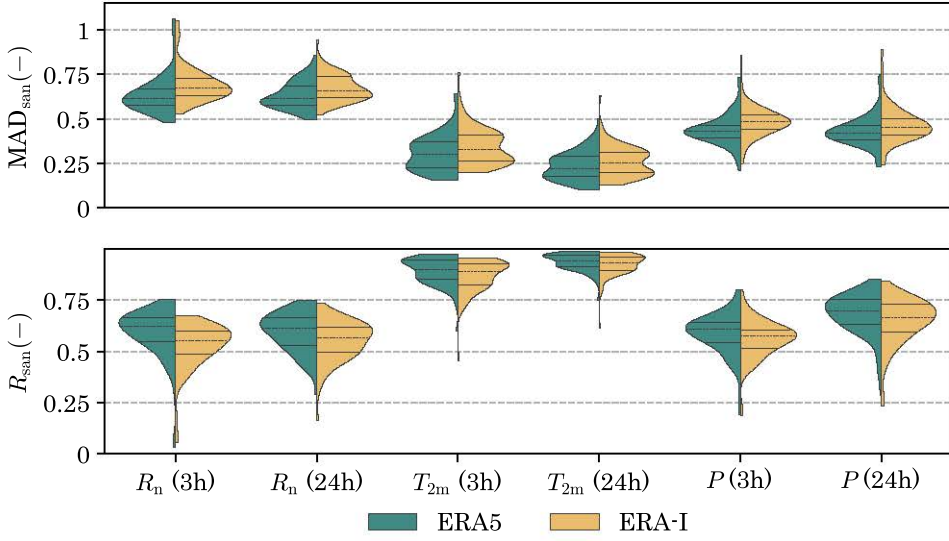


Figure C.5: Violin plots of temporal validation statistics of the surface net radiation (R_n), 2-meter air temperature (T_{2m}), and total precipitation (P) from ERA5 (green) and ERA-I (yellow). Statistics are calculated against in situ eddy-covariance measurements at both 3-hourly and daily temporal resolutions. Violin plots represent the distribution of the individual validation statistics with indication of the median and inter-quartile range and are calculated using a kernel density estimation approach. Statistics include the Mean Absolute Difference (MAD_{san} , standardised anomaly in situ time series from 83 sites as reference) and the Pearson correlation coefficient (R_{san} , standardised anomaly in situ time series from 83 sites as reference).

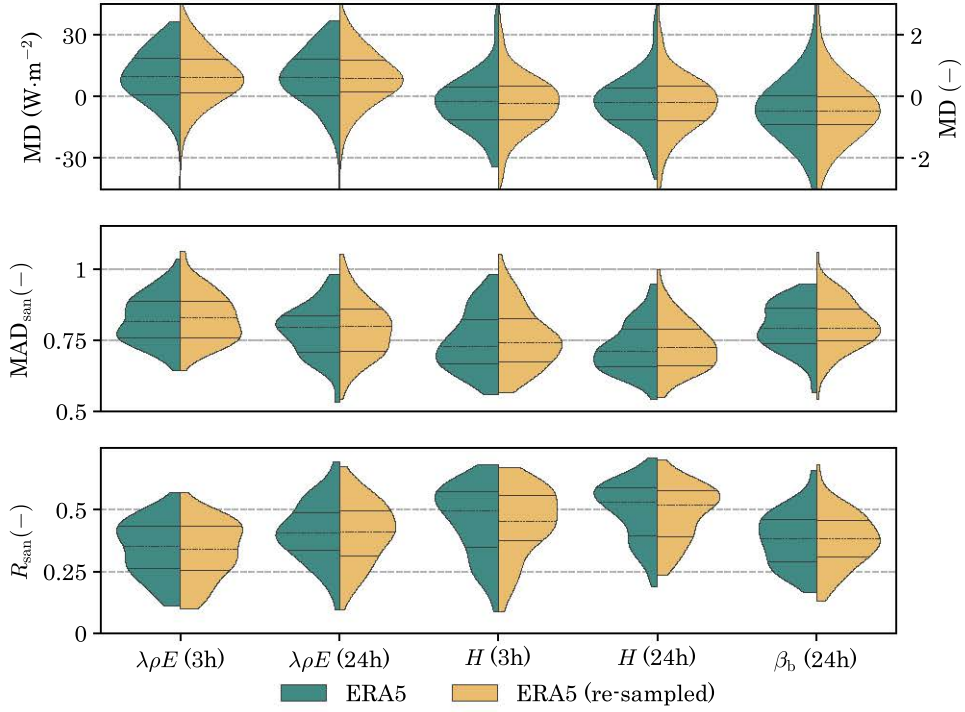


Figure C.6: Violin plots of temporal validation statistics of the surface latent heat flux ($\lambda\rho E$), surface sensible heat flux (H), and Bowen ratio (β_b) from ERA5 (green) and ERA5 linearly re-sampled to the spatial grid of ERA-I (yellow). Statistics are calculated against in situ eddy-covariance measurements at both 3-hourly and daily temporal resolutions. Violin plots represent the distribution of the individual validation statistics with indication of the median and inter-quartile range and are calculated using a kernel density estimation approach. Statistics include the Mean Difference (MD, raw in situ time series from 143 sites as reference), Mean Absolute Difference (MAD_{san}, standardised anomaly in situ time series from 77 sites as reference), and the Pearson correlation coefficient (R_{san} , standardised anomaly in situ time series from 77 sites as reference). For MD, the distribution of β_b is plotted on the right y-axis.

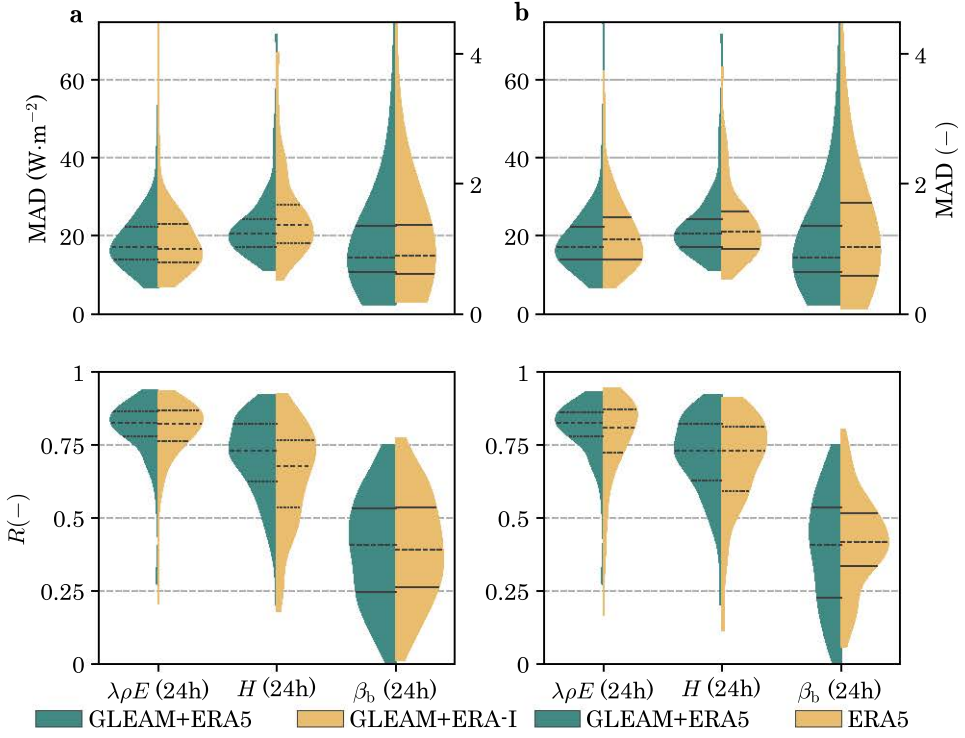


Figure C.7: Violin plots of temporal validation statistics of the surface latent heat flux ($\lambda\rho E$), surface sensible heat flux (H), and Bowen ratio (β_b) from GLEAM+ERA5, GLEAM+ERA-I, and ERA5. (a) compares the violin plots from GLEAM+ERA5 and GLEAM+ERA-I and (b) directly compares the violin plots from GLEAM+ERA5 and ERA5. Statistics are calculated against in situ eddy-covariance measurements at daily temporal resolution. Violin plots represent the distribution of the individual validation statistics with indication of the median and inter-quartile range and are calculated using a kernel density estimation approach. Statistics include the Mean Absolute Difference (MAD, raw in situ time series from 143 sites as reference) and the Pearson correlation coefficient (R , raw in situ time series from 143 sites as reference). For MAD, the distribution of β_b is plotted on the right y-axis.

C.3 Supplementary figures for Chapter 6

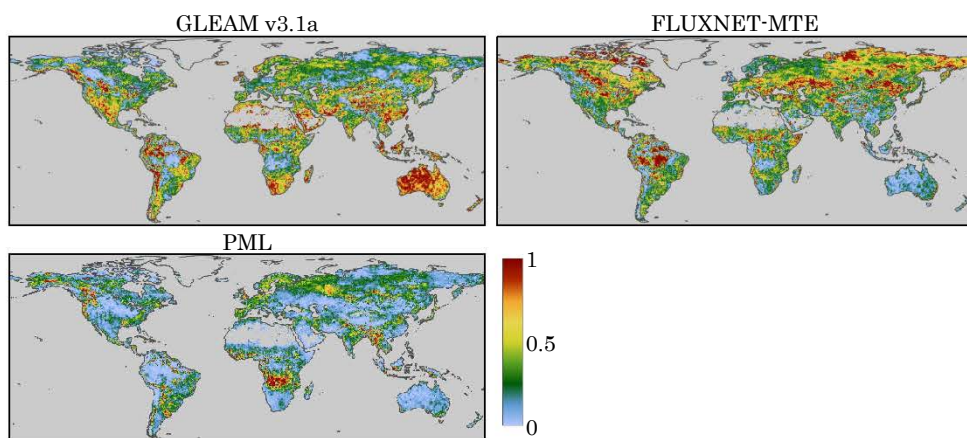


Figure C.8: Weights attributed to each of the data sets of terrestrial evaporation in the merging. Weights are calculated using the inverse variance technique, where the variance of the respective error distributions is estimated using a TCA.

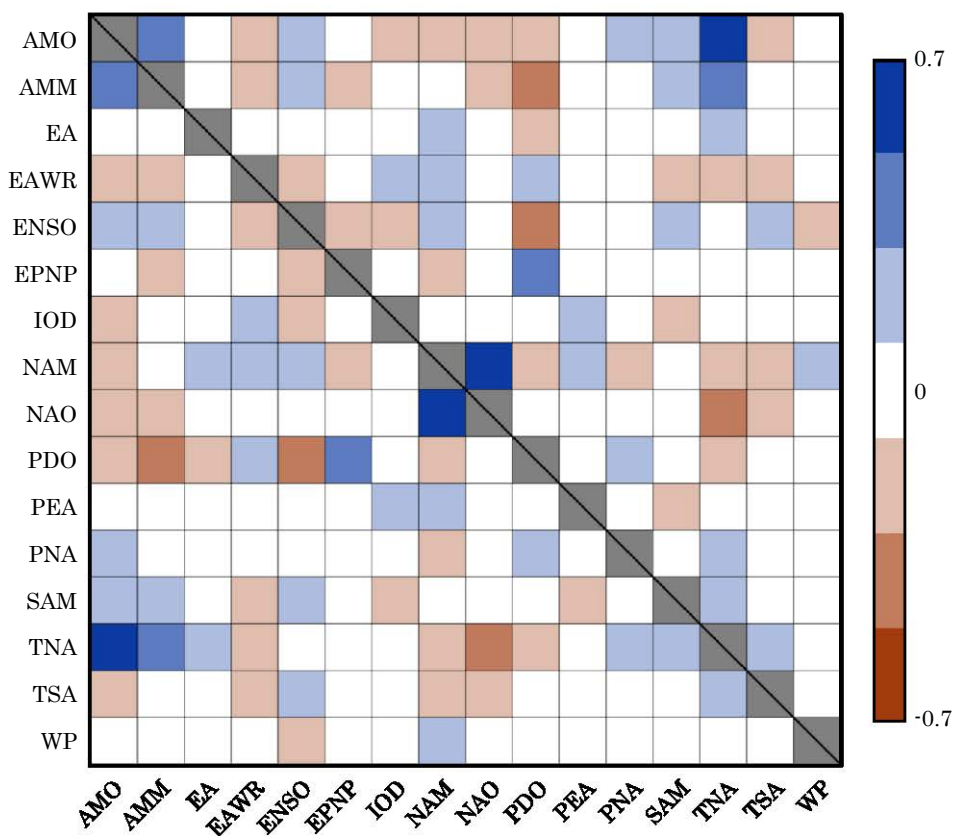


Figure C.9: Pearson correlation matrix of the 16 selected CIs. Statistically non-significant correlations ($p > 0.05$) – calculated using a two-sided Student's t-test – are set to zero, and the diagonal values are masked.

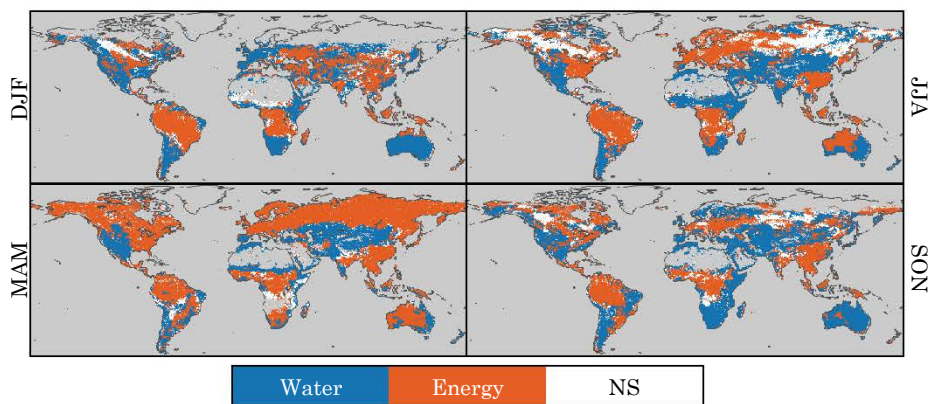


Figure C.10: Primary drivers of terrestrial evaporation. Classification is obtained by ranking the regression coefficients from the LASSO model targeting the anomalies of terrestrial evaporation based on the anomalies of precipitation and net radiation. Pixels where the regression coefficient for precipitation is top-ranked are classified as water-driven, whereas pixels where the regression coefficient for radiation is top-ranked are classified as energy-driven. NS indicates non-significant pixels.

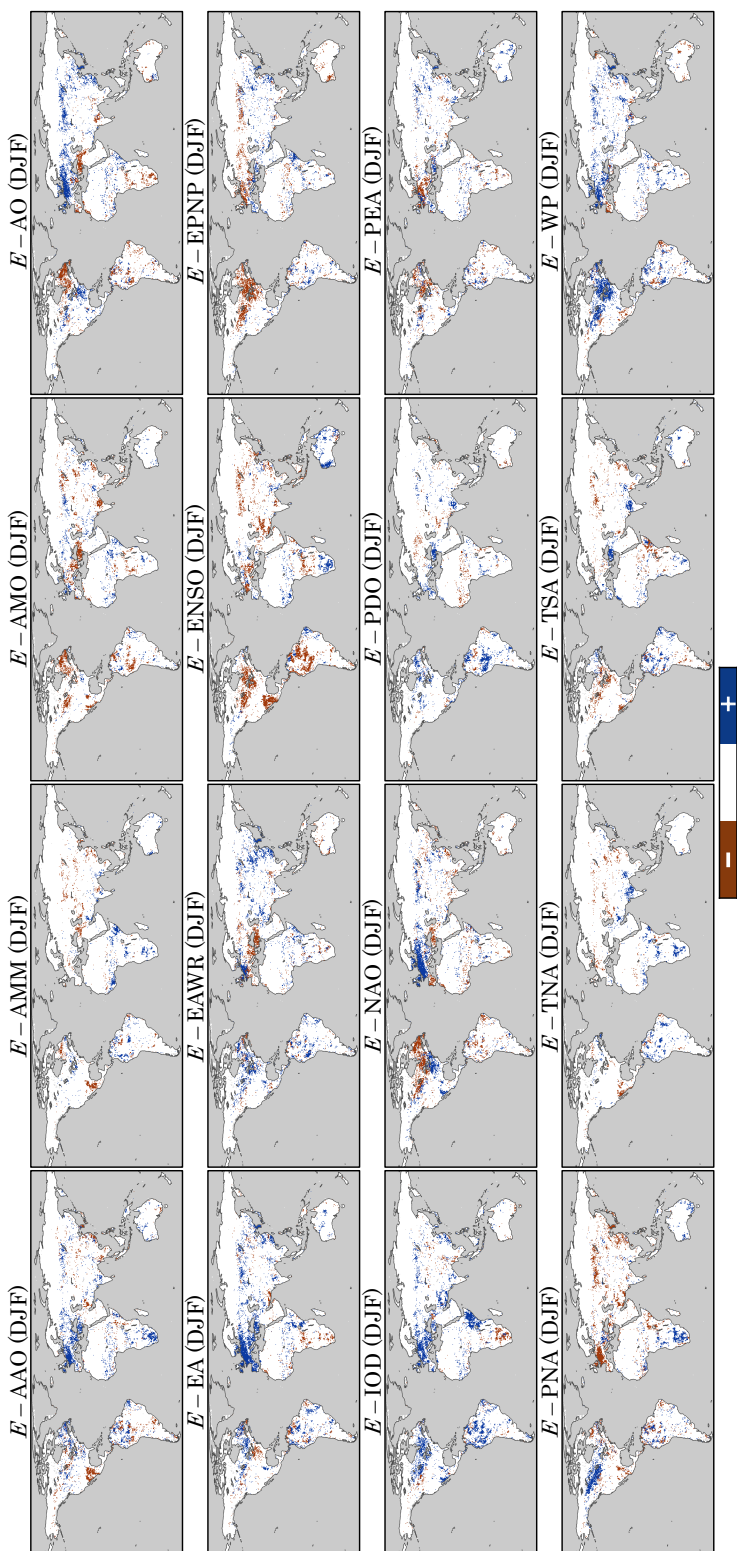


Figure C.11: Impact of teleconnections on the dynamics of terrestrial evaporation for December-January-February (DJF). Maps display the regions where the mode of variability affects terrestrial evaporation (i.e. the corresponding CI has a regression coefficient > 0 in the LASSO model), and the sign indicates the direction of the relation between the CI, and the variability in terrestrial evaporation. Regression coefficients corresponding to different lags introduced in each CI were summed to assess the overall impact per CI.

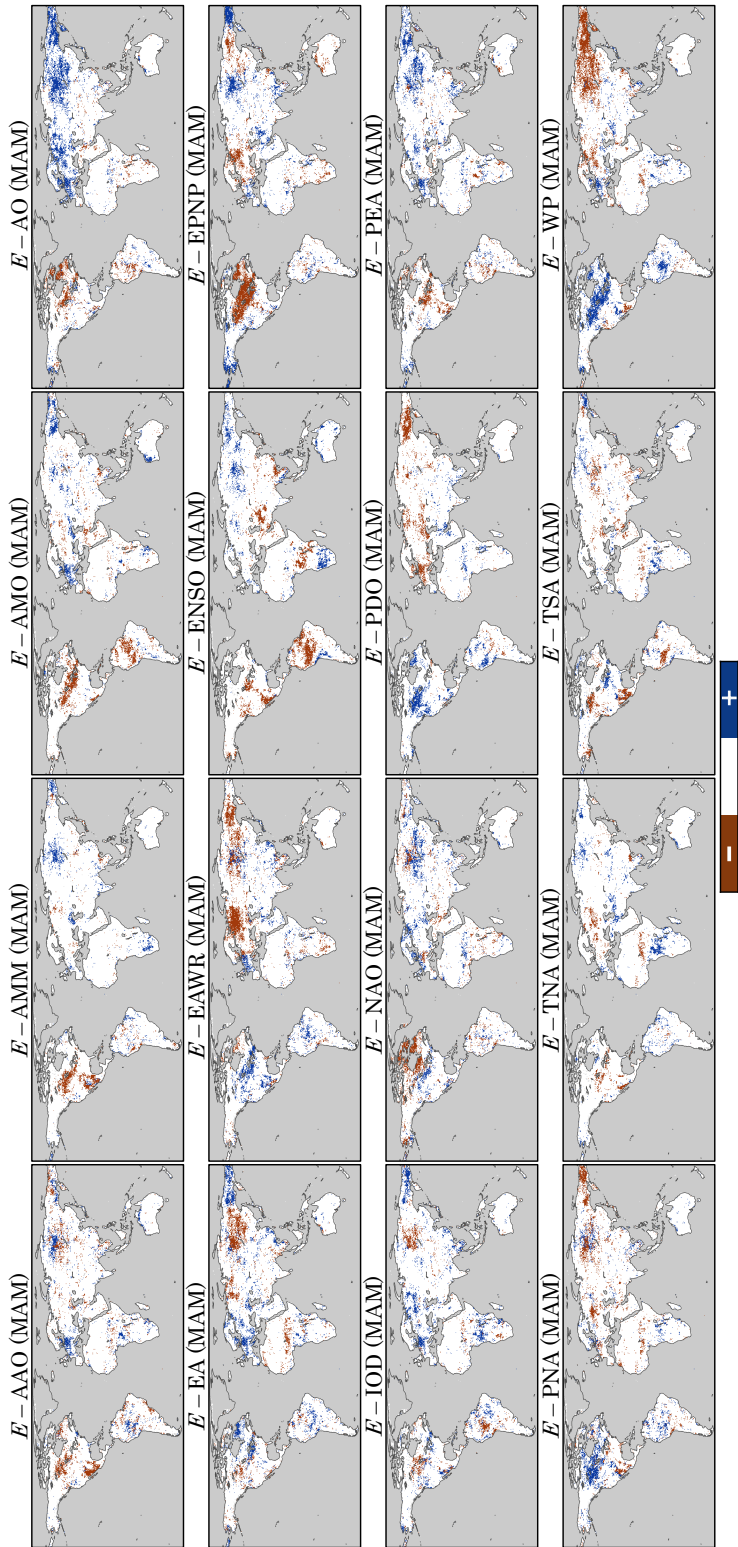


Figure C.12: Like Figure C.11 but for March-April-May (MAM).

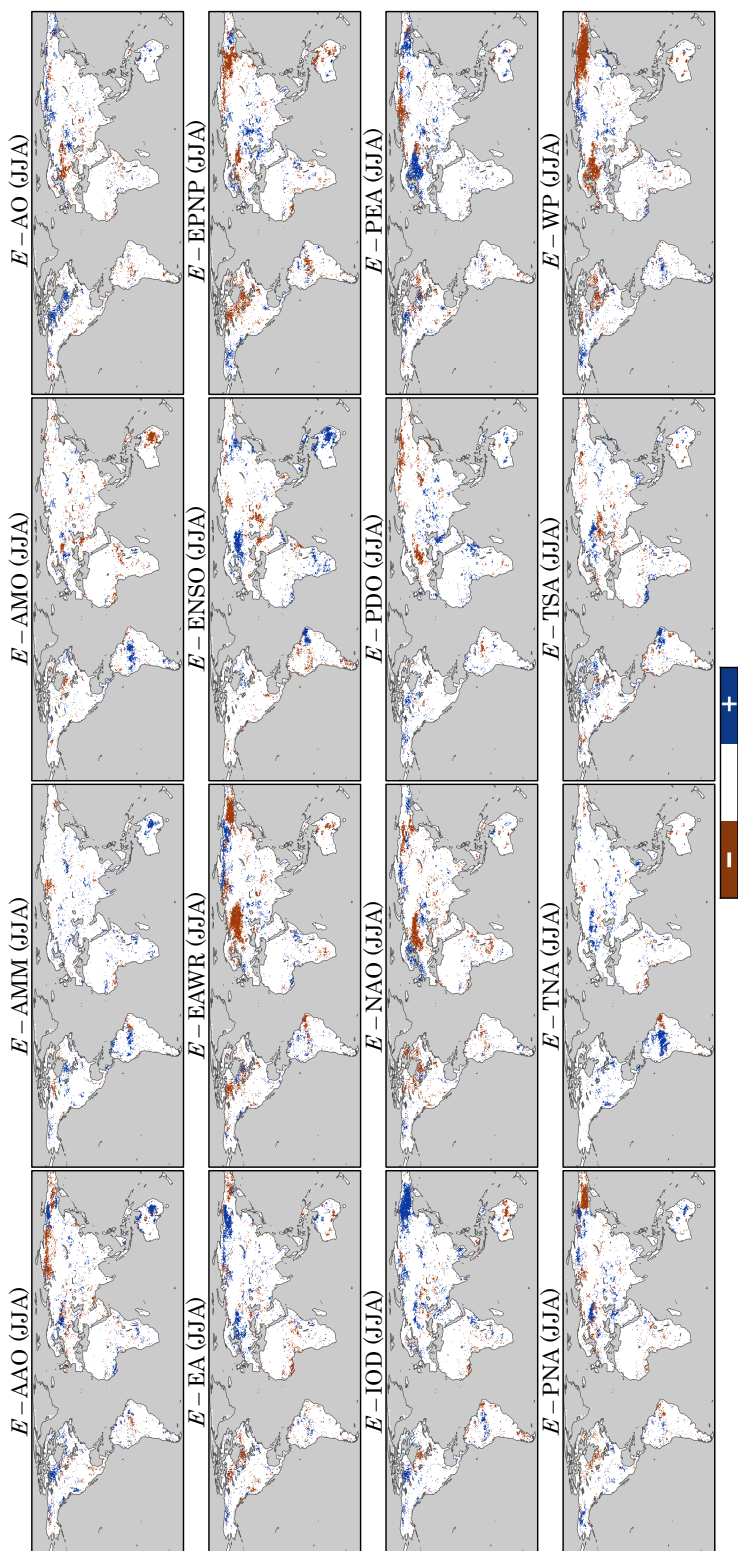


Figure C.13: Like Figure C.11 but for June-July-August (JJA).

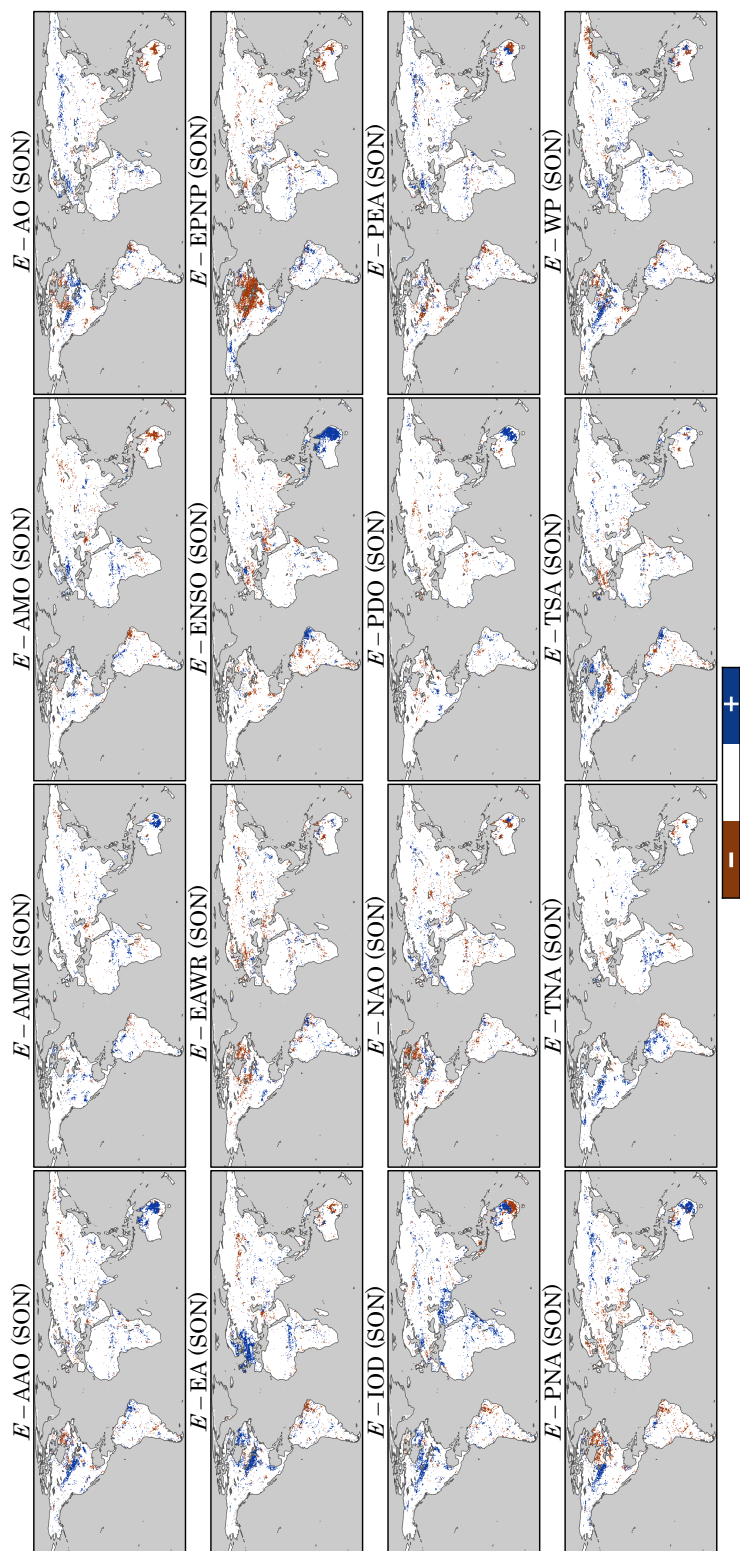


Figure C.14: Like Figure C.11 but for September-October-November (SON).

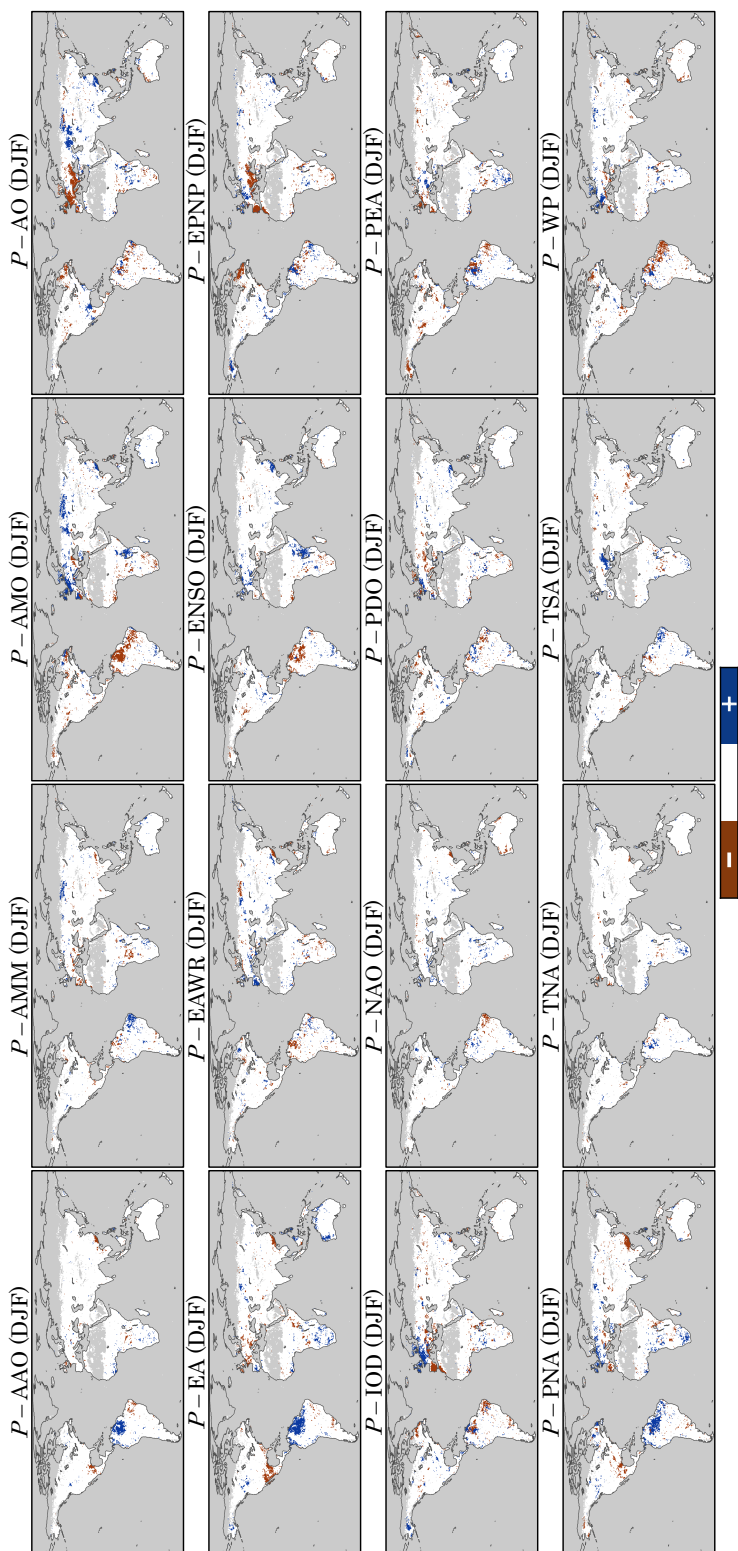


Figure C.15: Like Figure C.11 but for precipitation.

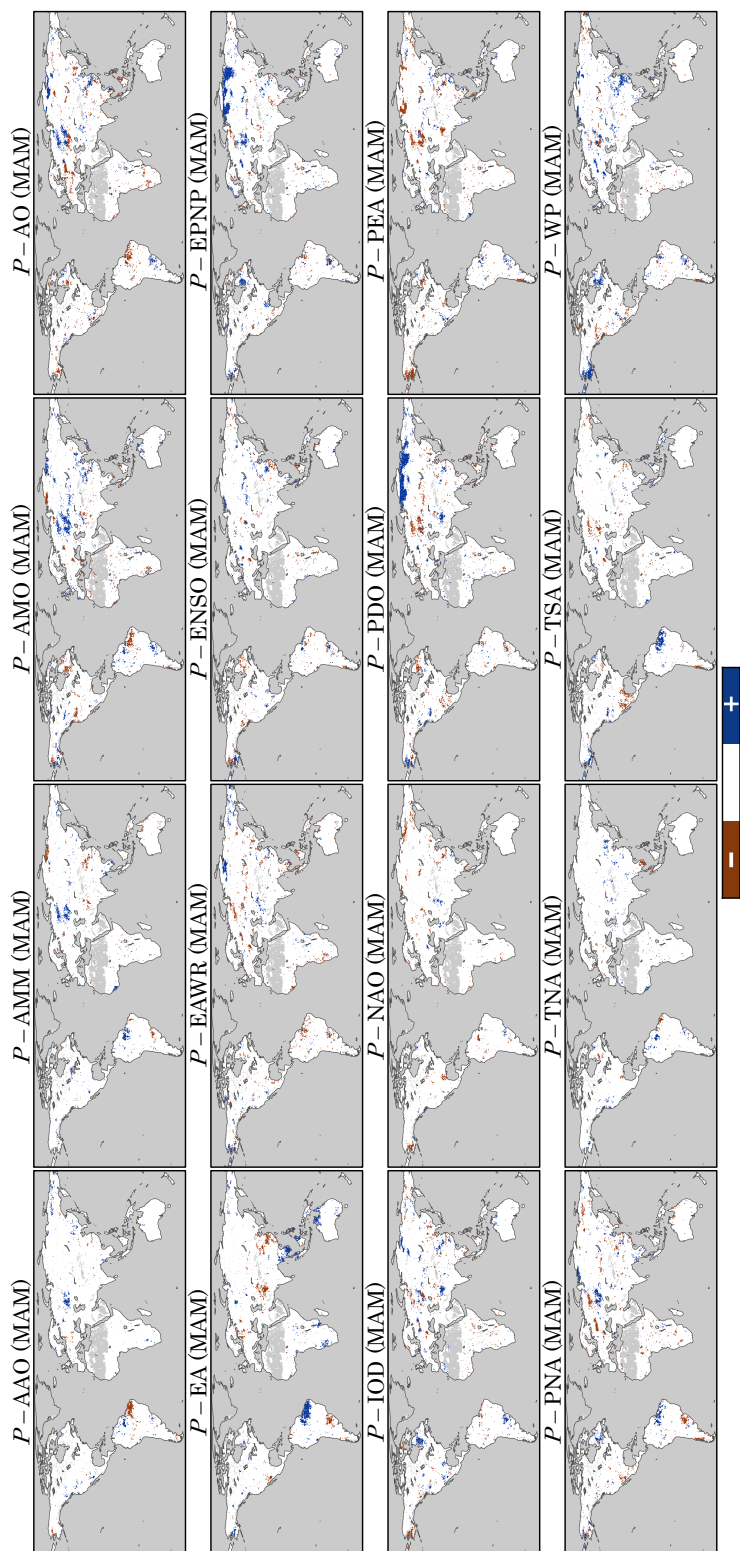


Figure C.16: Like Figure C.15 but for March-April-May (MAM).

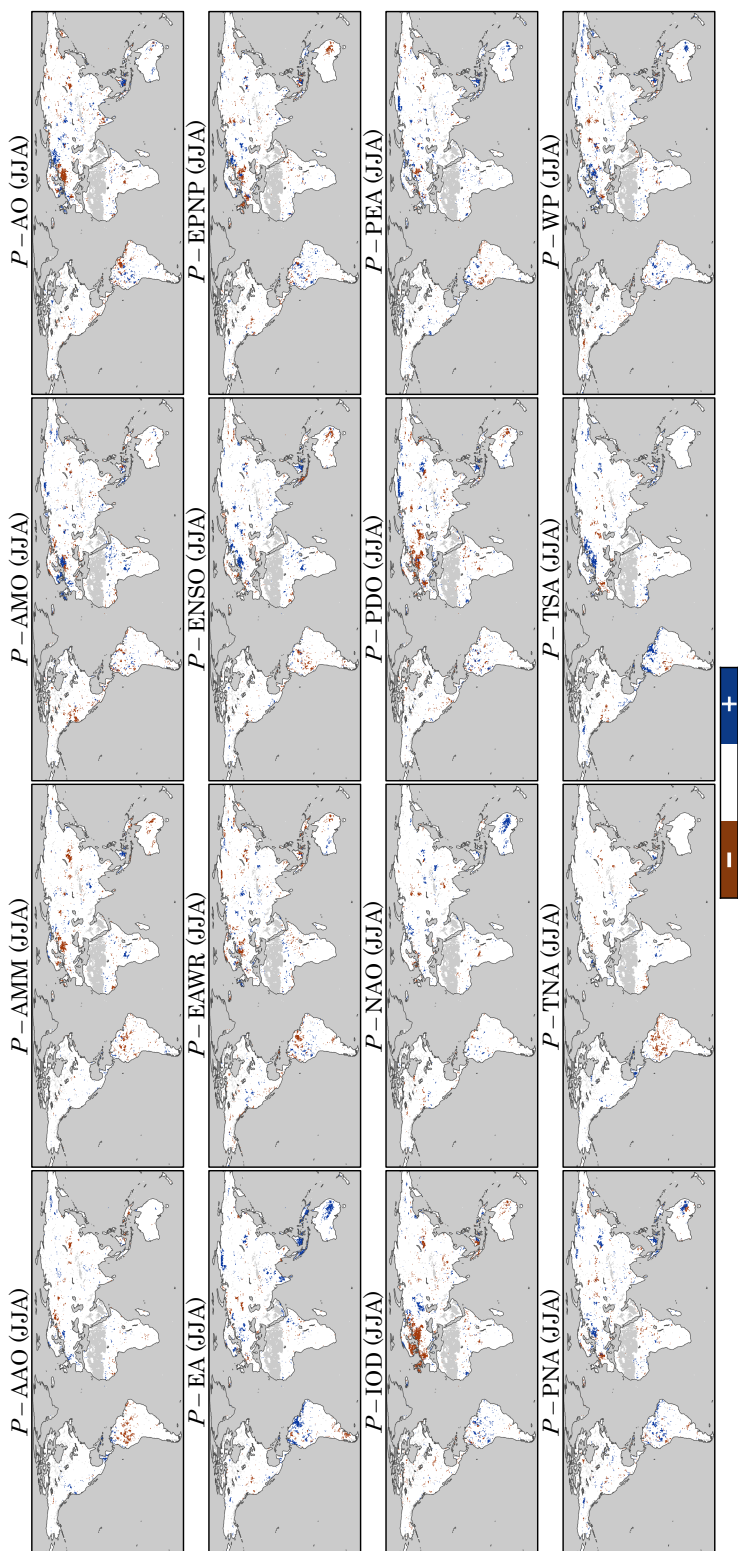


Figure C.17: Like Figure C.15 but for June-July-August (JJA).

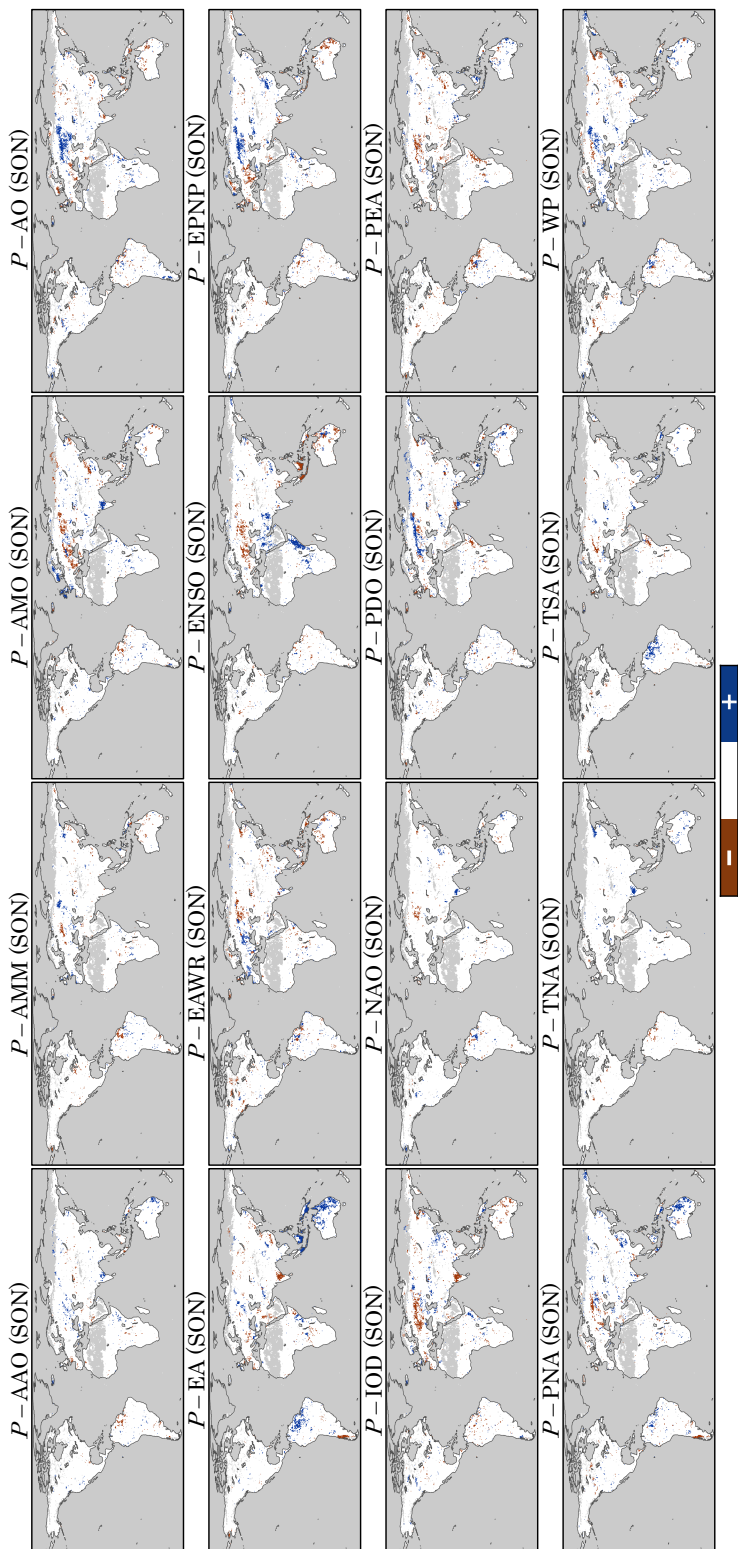


Figure C.18: Like Figure C.15 but for September-October-November (SON).

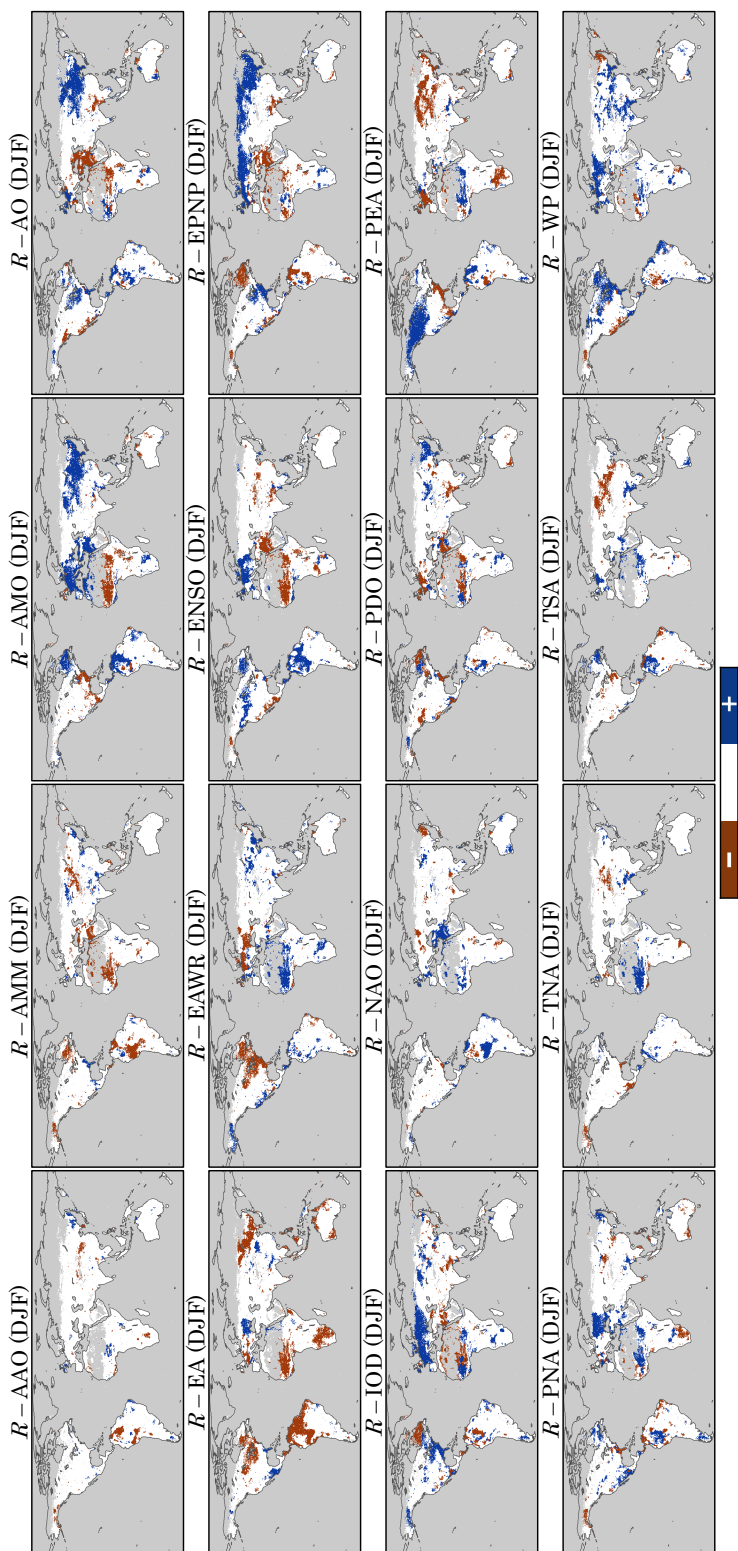


Figure C.19: Like Figure C.11 but for total incoming radiation.

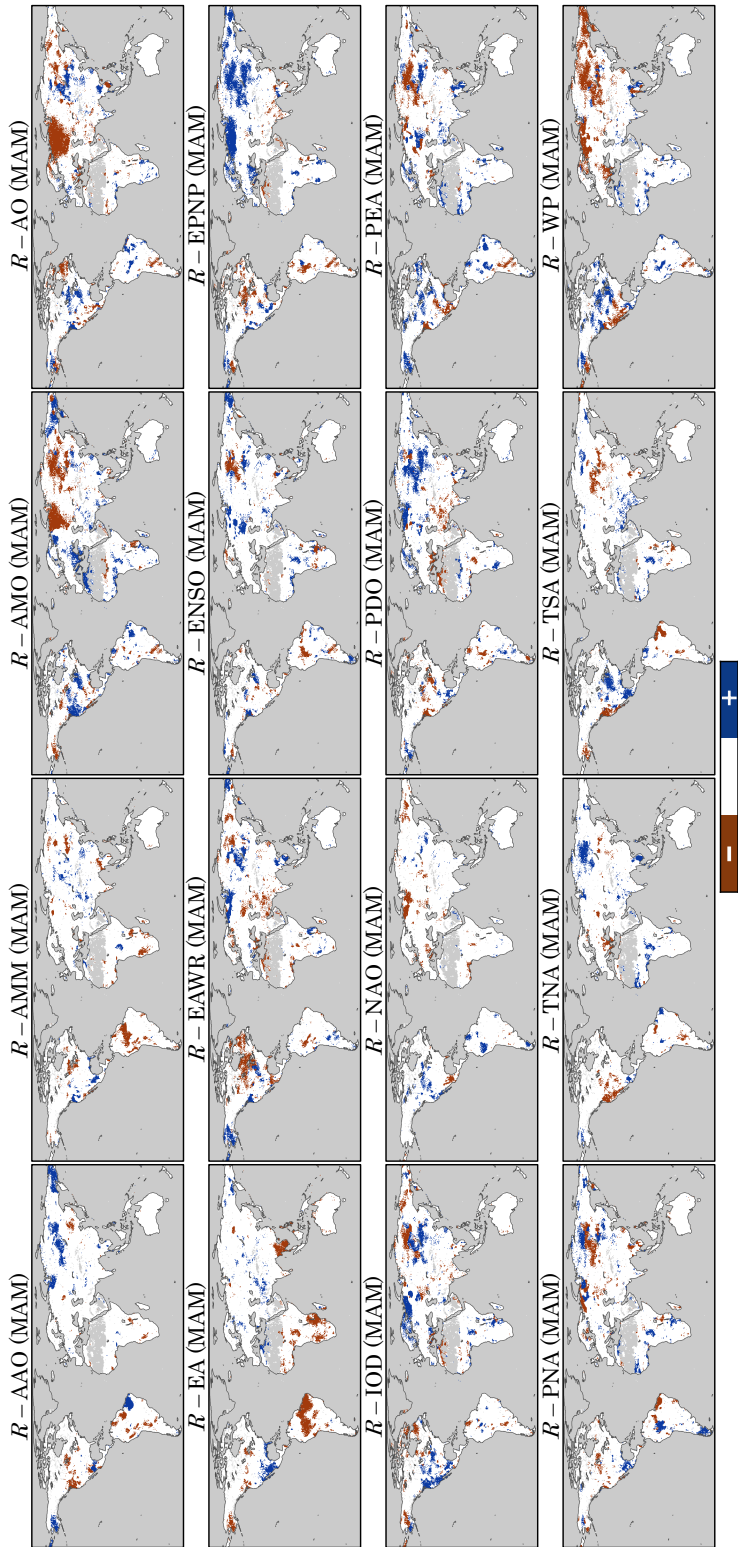


Figure C.20: Like Figure C.19 but for March-April-May (MAM).

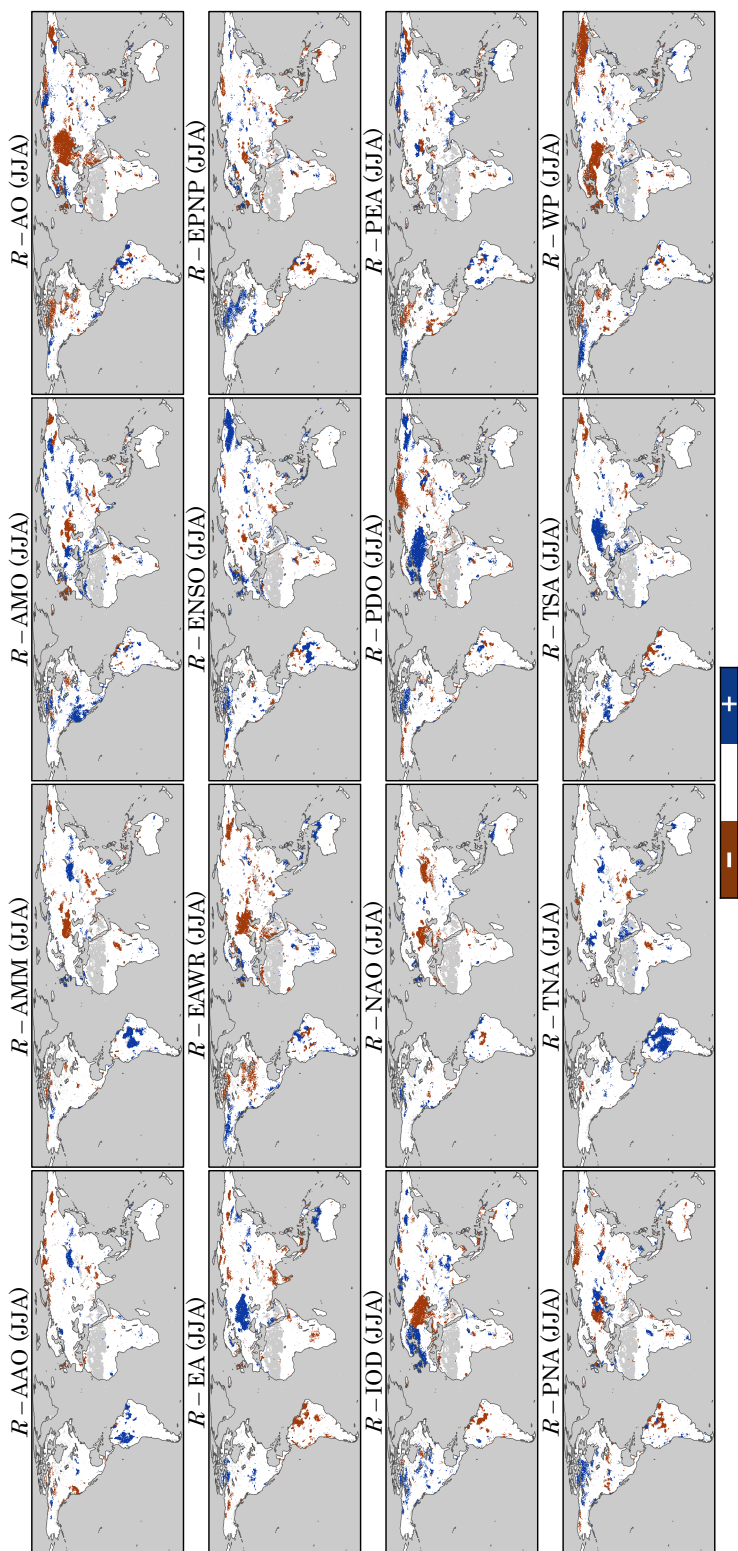


Figure C.21: Like Figure C.19 but for June-July-August (JJA).

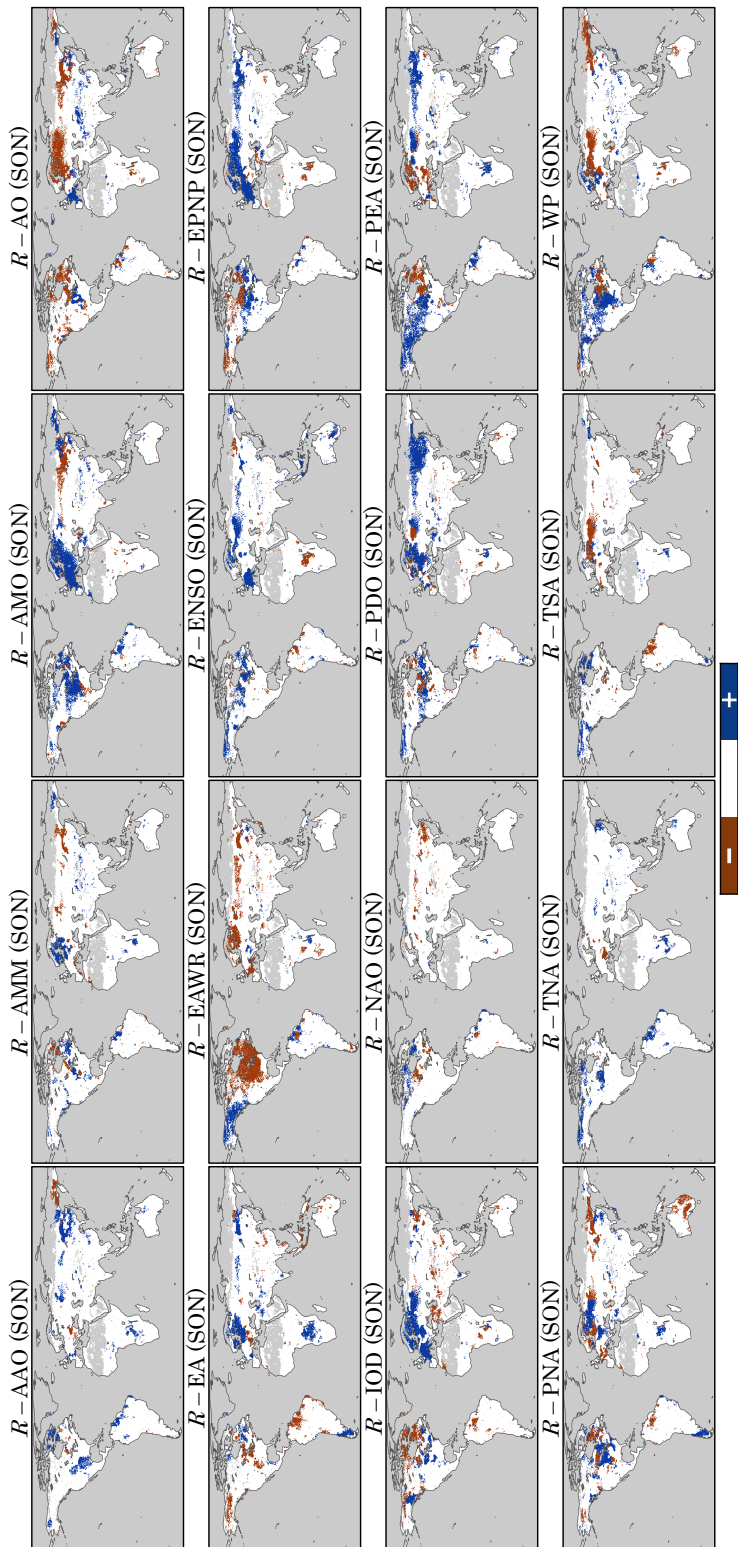


Figure C.22: Like Figure C.19 but for September-October-November (SON).

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Education (Ghent University)

2012–2019 Doctoral School of Bioscience Engineering

2010–2012 Master of Bioscience Engineering: Land and Water Management
Dissertation: Validation of radar-based precipitation measurements over Flanders (in Dutch)

2007–2010 Bachelor of Bioscience Engineering: Land and Forest Management
Dissertation: Alternative calibration methods for hydrological models: a critical analysis (in Dutch)

Training

2018 Multivariate statistics

2018 Deep Learning Specialization

2017 Machine Learning

2017 Deep Learning using a Convolutional Neural Network

2017 Introduction to Machine Learning Algorithms

2015 Advanced Academic English: Writing a Research Article

2015 Bayesian statistics

2014 Copula for Hydrology & Climate Application
2013 Basisassistententraining (*Training for teaching assistants*)
2013 Getting Started with High Performance Computing
2013 Introduction to R: an Open-Source Statistical Toolbox
2012 First SMOS Training Course

Employment

2014–2019 Teaching Assistant – Ghent University
2014–2019 Doctoral Researcher – Ghent University
2012–2014 Scientific Researcher – Ghent University

Teaching Experience (Ghent University)

2019 Hydrological Processes and Hydrometry (exercises, *in Dutch*)
2017 Geographical Information Systems (exercises partim Hydrology)
2015–2018 Hydrology and Meteorology (exercises partim Hydrology, *in Dutch*)
2014–2019 Irrigation and Drainage (exercises partim Drainage)
2014–2019 Hydrological Modelling (exercises)
2014–2019 Groundwater Flow (exercises)

Tutor of Master Thesis Dissertations

2018–2019 Emma Tronquo. Linking droughts to ocean-atmospheric oscillations. Supervisor: Miralles, D.G.
2017–2018 Dries Mergaert. Investigating the impact of ocean-atmospheric oscillations on tree-ring width using a simple supervised learning method. Supervisor: Miralles, D.G.
2016–2017 Stefanie Coppens. Comparing two data assimilation algorithms for incorporating satellite-based soil moisture observations into a hydrological model (*in Dutch*). Supervisors: Verhoest, N.E.C & Lievens, H.
2015–2016 Jeroen Claessen. Optimization of the roughness module in the Land Parameter Retrieval Model (LPRM) for improved soil moisture estimation (*in Dutch*). Supervisors: Verhoest, N.E.C & Lievens, H.
2013–2014 Sofie Baeyens. Comparing different conceptual rainfall-runoff models for simulating extreme discharges (*in Dutch*). Supervisor: Verhoest, N.E.C.

2013–2014 Gemma Casas Papell. Assessment of Bartlett-Lewis stochastic rainfall models for preserving modelled low flow. Supervisor: Verhoest, N.E.C.

Peer-reviewed publications

Published

Claessen, J., **Martens, B.**, Detto, M., Molini, A., Demuzere, M., Miralles, D.G., 2019. Global biosphere–climate interaction: a multi-scale appraisal of observations and models. *Biogiosciences*, *accepted for publication*.

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Miralles, D.G., **Martens, B.**, Beck, H.E., Dolman, A.J., Jimnez, C., McCabe, M.F., Wood, E.F., 2019. Land evaporation. *Bulletin of the American Meteorological Society* (in: *State of the Climate in 2018*) 100 (9), S40–S41.

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Martens, B., Waegeman, W., Dorigo, W.A., Verhoest, N.E.C., Miralles, D.G., 2018. Terrestrial evaporation response to modes of climate variability. *npj Climate and Atmospheric Science* 1 (1), 43.

Martens, B., de Jeu, R.A.M., Verhoest, N.E.C., Schuurmans, H., Kleijer, J., Miralles, D.G., 2018. Towards estimating land evaporation at fields scales using GLEAM. *Remote Sensing* 10 (11), 1720.

Talsma, C.J., Good, S.P., Miralles, D.G., Fisher, J.B., **Martens, B.**, Jiménez, C., Purdy, A.J., 2018. Sensitivity of evapotranspiration components in remote sensing-based models. *Remote Sensing*, 10 (10) 1601.

Jiménez, C., **Martens, B.**, Miralles, D.G., Fisher, J.B., Tu, K., Beck, H.E., Fernández-Prieto, D., 2018. Exploring the merging of the global land evaporation WACMOS-ET products on local tower measurements. *Hydrology and Earth System Sciences* 22 (8), 4513–4533.

Meier, R., Davin, E.L., Lejeune, Q., Hauser, M., Li, Y., **Martens, B.**, Schultz, N.M., Sterling, S., Thiery, W., 2018. Evaluating and improving the Community Land Models sensitivity to land cover. *Biogeosciences* 15 (15), 4731–4757.

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Talsma, C.J., Good, S.P., Jiménez, C., **Martens, B.**, Fisher, J.B., Miralles, D.G., McCabe, M.F., Purdy, A.J., 2018. Partitioning of evapotranspiration in remote sensing-based models. *Agriculture and Forest Meteorology* 260–261 (10), 131–143.

Miralles, D.G., **Martens, B.**, Beck, H.E., Dolman, A.J., Jiménez, C., McCabe, M.F., Wood, E.F., 2017. Land evaporation. *Bulletin of the American Meteorological Society* (in: *State of the Climate in 2016*) 98 (8), S34–S35.

Martens, B., Miralles, D.G., Lievens, H., van der Schalie, R., de Jeu, R.A.M., Fernández-Prieto, D., Beck, H.E., Dorigo, W.A., Verhoest, N.E.C., 2017. GLEAM v3: satellite-based land evaporation and root-zone soil moisture. *Geoscientific Model Development* 10 (5), 1903–1925.

Beck, H.E., van Dijk, A.I.J.M., Levizzani, V., Schellekens, J., Miralles, D.G., **Martens, B.**, de Roo, A., 2017. MSWEP: 3-hourly 0.25° global gridded precipitation (1979–2015) by merging gauge, satellite, and reanalysis data. *Hydrology and Earth System Sciences* 21 (1), 589–615.

Lievens, H., **Martens, B.**, Verhoest, N.E.C., Hahn, S., Miralles, D.G., 2017. Assimilation of global radar backscatter and radiometer brightness temperature observations to improve soil moisture and land evaporation estimates. *Remote Sensing of Environment* 189 (2), 194–210.

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Lievens, H., De Lannoy, G.J.M., Al Bitar, A., Drusch, M., Dumedah, G., Hendricks-Franssen, H.-J., Kerr, Y.H., Tomer, S., **Martens, B.**, Merlin, O., Pan, M., Roundy, J.K., Vereecken, H., Walker, J.P., Wood, E.F., Verhoest, N.E.C., Pauwels, V.R.N., 2016. Assimilation of SMOS soil moisture and brightness temperature products into a land surface model. *Remote Sensing of Environment* 180 (7), 292–304.

Martens, B., Miralles, D.G., Lievens, H., Fernández-Prieto, D., Verhoest, N.E.C., 2016. Improving terrestrial evaporation estimates over continental Australia through assimilation of SMOS soil moisture. *International Journal of Applied Earth Observation and Geoinformation* 48 (6), 146–162.

Miralles, D.G., Jiménez, C., Jung, M., Michel, D., Ershadi, A., McCabe, M.F., Hirschi, M., **Martens, B.**, Dolman, A.J., Fisher, J.B., Mu, Q., Seneviratne, S.I., Wood, E.F., Fernández-Prieto, D., 2016. The WACMOS-ET project – Part 2: Evaluation of global terrestrial evaporation datasets. *Hydrology and Earth System Sciences* 20 (2), 823–842.

Michel, D., Jiménez, C., Miralles, D.G., Jung, M., Hirschi, M., Ershadi, A., **Martens, B.**, McCabe, M.F., Fisher, J.B., Mu, Q., Seneviratne, S.I., Wood,

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Lievens, H., Kumar Tomer, S., Al Bitar, A., De Lannoy, G.J.M., Drusch, M., Dumedah, G., Hendricks-Franssen, H.-J., Kerr, Y.H., **Martens, B.**, Pan, M., Roundy, J.K., Vereecken, H., Walker, J.P., Wood, E.F., Verhoest, N.E.C., Pauwels, V.R.N., 2015. SMOS soil moisture assimilation for improved hydrologic simulation in the Murray Darling Basin, Australia. *Remote Sensing of Environment* 168 (10), 146–162.

Lievens, H., Al Bitar, A., Verhoest, N.E.C., Cabot, F., De Lannoy, G.J.M., Drusch, M., Dumedah, G., Hendricks-Franssen, H.J., Kerr, Y., Kumar Tomer, S., **Martens, B.**, Merlin, O., Pan, M., van den Berg, M.J., Vereecken, H., Walker, J.P., Wood, E.F., Pauwels, V.R.N., 2015. Optimization of a radiative transfer operator for simulating SMOS brightness temperatures over the Upper Mississippi Basin, USA. *Journal of Hydrometeorology* 16 (3), 1109–1134.

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In review

Maes, W.H., Miralles, D.G., Pagán, B., **Martens, B.**, Gentine, P., Steppe, K., Verhoest, N.E.C., Dorigo, W.A., 2019. Ecosystem evaporation closely linked to sun-induced fluorescence as evidenced by satellite data and radiative transfer models. *Remote Sensing of Environment*.

Martens, B., Schumacher, D.L., Wouters, H., Muñoz-Sabater, J., Verhoest, N.E.C., Miralles, D.G., 2019. Evaluating the surface energy partitioning in ERA5. *Geoscientific Model Development Discussions*.

Conference proceedings

Claessen, J., **Martens, B.**, Verhoest, N.E.C., Molini, A., Miralles, D.G., 2017. Global climatic drivers of vegetation based on wavelet analysis. In 2017 9th International Workshop on the Analysis of Multitemporal Remote Sensing Images (MultiTemp), IEEE.

Martens, B., Miralles, D.G., Dorigo, W.A., Waegeman, W., Verhoest, N.E.C., 2017. Investigating the control of ocean-atmospheric oscillations over global terrestrial evaporation using a simple supervised learning method. In 2017 9th International Workshop on the Analysis of Multitemporal Remote Sensing Images (MultiTemp), IEEE.

Martens, B., Lievens, H., Walker, J.P., Panciera, R., Tanase, M., Monerris, A., Gao, Y., Wu, X., Verhoest, N.E.C., 2013. An alternative roughness parameterization for soil moisture retrievals from passive microwave Observations. In ESA Living Planet Symposium, Proceedings. European Space Agency (ESA).

Conference presentations (only first author)

Martens, B., Lievens, H., Verhoest, N.E.C., Miralles, D.G., 2019. Assimilation of satellite-based geophysical variables to improve land evaporation estimates. European Geosciences Union General Assembly 2019. Invited oral presentation.

Martens, B., de Jeu, R.A.M., Verhoest, N.E.C., Schuurmans, H., Kleijer, J., Miralles, D.G., 2019. Estimating land evaporation at field scales using GLEAM. European Geosciences Union General Assembly 2019. PICO presentation.

Martens, B., Waegeman, W., Dorigo, W.A., Verhoest, N.E.C., Miralles, D.G., 2017. Investigating the control of ocean-atmospheric oscillations on global terrestrial evaporation. American Geosciences Union Fall Meeting 2017. Oral presentation.

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