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**Using real-time observations and land  
surface modelling for improved irrigation  
and water resources management in  
Mediterranean climate**

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Dissertation

zur

Erlangung des Doktorgrades (Dr. rer. nat.)

der

Mathematisch-Naturwissenschaftlichen Fakultät

der

Rheinischen Friedrich-Wilhelms-Universität Bonn

vorgelegt von

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Berlin

Bonn, November 2023



Angefertigt mit Genehmigung der Mathematisch-Naturwissenschaftlichen Fakultät  
der Rheinischen Friedrich-Wilhelms-Universität Bonn

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Tag der Promotion: 28.03.2024

Erscheinungsjahr: 2024



# Abstract

Irrigated agriculture is essential to sustain crop production and livelihoods of the rural population in semi-arid and arid regions such as the Mediterranean. Meanwhile, unsustainable irrigation practices, population growth, and climate change are increasing agricultural water demand while exacerbating water scarcity. Effective measures to reduce agricultural water consumption while sustaining a high level of crop production and securing environmental sustainability are therefore urgently needed.

This thesis aims at increasing the availability of environmental data and advancing the representation of agricultural systems in land surface models to improve local and regional scale irrigation and water resources management in the Mediterranean.

In the first part, the use of a low-cost weather station to deliver reliable and timely data for environmental monitoring, research, and modelling is assessed. Performance and data quality of multiple stations are examined in terms of inter-sensor variability and in comparison to a high-performance weather station.

The second part of this thesis focusses on improving the representation of typical Mediterranean crops in the Community Land Model version 5. A new sub-model to model deciduous fruit orchards is developed encompassing crop phenological stages, biomass growth and partitioning into different plant organs as well as typical management practices. The development is then tested using extensive field measurements from an apple orchard.

Finally, the new sub-model is used to assess irrigation and water management in a small Greek catchment dominated by irrigated apple orchards. First, simulated crop growth and soil moisture dynamics are examined in relation to irrigation and compared to observations from two monitored apple orchards. Thereby, further model improvements are made to represent the local irrigation practices. Subsequently, the model is applied at regional scale to determine irrigation requirements and examine the impact of different irrigation deficit scenarios on yield and crop water use efficiency as well as to assess the water saving potential in the catchment.



# Zusammenfassung

Bewässerung sichert die landwirtschaftliche Produktion sowie die Lebensgrundlage der ländlichen Bevölkerung in semiariden und ariden Regionen wie dem Mittelmeerraum. Gleichzeitig erhöhen nicht nachhaltige Bewässerungspraktiken, Bevölkerungswachstum und der Klimawandel den landwirtschaftlichen Wasserbedarf und verschärfen die Wasserknappheit. Wirkungsvolle Maßnahmen zur Reduzierung des landwirtschaftlichen Wasserverbrauchs bei gleichzeitiger Erhaltung der Ernten und Gewährleistung ökologischer Nachhaltigkeit sind daher dringend erforderlich.

Die vorliegende Dissertation hat zum Ziel, die Verfügbarkeit von Umweltdaten zu erhöhen und die Darstellung landwirtschaftlicher Systeme in Landoberflächenmodellen weiterzuentwickeln, um Bewässerung und Wasserressourcenmanagement im Mittelmeerraum auf lokaler und regionaler Skala zu verbessern.

Im ersten Teil wird die Verwendung einer kosteneffektiven Wetterstation zur Bereitstellung zuverlässiger und aktueller Daten für Umweltmessungen, Forschung und Modellierung untersucht. Die Eignung und Datenqualität mehrerer Stationen werden hinsichtlich der Variabilität zwischen einzelnen Sensoren sowie im Vergleich zu einer hochwertigen Wetterstation bewertet.

Der zweite Teil dieser Dissertation befasst sich mit der Verbesserung der Darstellung typischer mediterraner Nutzpflanzen im Community Land Model Version 5. Ein neues Submodell zur Modellierung von sommergrünen Obstplantagen wird entwickelt, welches die phänologischen Entwicklungsphasen, das Wachstum und die Aufteilung der Biomasse auf verschiedene Pflanzenorgane sowie typische Bewirtschaftungspraktiken umfasst. Die Modellentwicklung wird anschließend anhand umfangreicher Feldmessungen von einer Apfelplantage getestet.

Schließlich wird das neue Submodell dazu verwendet, die Bewässerung und das Wasserressourcenmanagement in einem kleinen griechischen Einzugsgebiet zu untersuchen, in dem vorherrschend bewässerte Apfelplantagen gepflanzt sind. Dafür werden zuerst die Simulierung des Pflanzenwachstums und der Bodenfeuchtedynamik in

Bezug auf die Bewässerung untersucht und mit Messungen aus zwei Apfelplantagen verglichen. In dem Zusammenhang werden weitere Modellverbesserungen zur Darstellung lokaler Bewässerungspraktiken vorgenommen. Anschließend wird das Modell auf regionaler Skala angewendet, um den Bewässerungsbedarf zu bestimmen und die Auswirkungen unterschiedlicher Szenarien der Defizitbewässerung auf Ertrag und Wassernutzungseffizienz zu untersuchen sowie das Potenzial zur Wassereinsparung im Einzugsgebiet zu bewerten.



# Acknowledgements

First of all, I want to thank my supervisors at Forschungszentrum Jülich Heye Bogena and Harrie-Jan Hendricks Franssen for their time, guidance, and fruitful discussions over the past years. I am grateful for the opportunities this has given me and for the scientific knowledge I have gained during my time at IBG-3. A big thanks also goes to Cosimo Brogi for his continuous support and readiness to share his experience, exchange thoughts, and provide helpful feedback throughout my time as a PhD student.

I also want to thank our project partners in Greece Andreas Panagopoulos, Vassilis Pinaras, Anna Chatzi, Konstantinos Babakos, and Ioannis Tsakmakis. It has been a great pleasure working with them, in the field under the sizzling Greek sun or remotely. Thank you also to Stamatis and Nikos for working with us. Another thanks goes to Bernd Schilling and Ansgar Weuthen for their technical support and for teaching me to install SoilNet devices in the snow and mud as well as to Burkhard Neuwirth for sharing his knowledge about sapflow sensors.

Next, I would like to thank my fellow PhD students for helping each other out, for the useful exchange during group meetings, and relaxing lunch and coffee breaks. Thank you also to the administrative and other non-scientific staff at IBG-3. A special thanks to Chris for being a great teammate as PhD representatives and to Marie Ludwig for her work and motivation as scientific coordinator and for her constant support to the PhD students. Thanks also to Marius for many enjoyable car sharing rides.

Another thanks goes to Damiano Zanotelli from Bolzano University for a fruitful collaboration as well as to Sean Swenson and other folks at NCAR for their help, inspiring scientific exchange, and the wonderful time in Boulder.

Apart from everyone who has been part of my work life over the last years, I'm incredibly grateful for all the wonderful people in my life outside the PhD. A huge hug to Mia, Tschou, Caro, Lilith and the rest of the aerial silks crew for countless hours of training, having fun together, and taking my mind off of work when I needed it. Hugs to my lovely flatmates Anna, Alena, and Julian for sharing our lives, meals, laughs, kitchen hangouts,

and many joyful as well as difficult times. A big hug to Suse, Greta, Agata, Clara, Lotte, Inga, Caro, Vic, Leo, Max, Rhoda, Job, Albert, Sofi, Marina, and all the other old and new friends in Cologne and around the world for being in my life, doing remote co-working sessions together and staying connected. Thank you Antony for being the crazy human you are and for having been with me during part of this journey.

Hugs and kisses to Anna for being the best conversational partner, accepting me more than I accept myself, exploring our connection together, and for being just a wonderful person. I'm so happy to have you in my life.

Thank you to my parents, Eva and Tilman, for all your love, trust, support, open mindedness, and interest in anything I do. Thank you to my awesome sister Annah and to Jay for introducing me to EA and many mind-opening experiences. Thanks Sis for being such great company for festivals, travels, sports, and other adventures. You guys are the best family ever!

Finally, thank you Lorenz for becoming such an important part of my life in the final phase of my PhD. I love you for your endless enthusiasm and energy, your warmth, the best hugs in the world, for pushing me and supporting me, for not following the norm, and introducing me to a new world of music. Thank you for being a wonderful partner and for bringing a lot of glitter into my life. I'm excited to start a new chapter together •–

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# List of Abbreviations

|                                |   |
|--------------------------------|---|
| <b>%bias</b>                   | Percent bias  |
| <b><math>\mu</math></b>        | Arithmetic mean                                     |
| <b>BDT</b>                     | Broadleaf deciduous tree                            |
| <b>BGC-crop</b>                | Biogeochemistry crop module                         |
| <b>Biome-BGC</b>               | Biome BioGeochemical Cycles                         |
| <b>C</b>                       | Carbon  |
| <b>C1</b>                      | Official ICOS climate station Selhausen             |
| <b>CLM</b>                     | Community Land Model                                |
| <b>CM</b>                      | Crop model  |
| <b>CS</b>                      | Climate station                                     |
| <b>CWUE</b>                    | Crop water use efficiency                           |
| <b>DI</b>                      | Deficit irrigation                                  |
| <b>DSSAT</b>                   | Decision Support System for Agrotechnology Transfer |
| <b>EC</b>                      | Eddy covariance                                     |
| <b>ESDB</b>                    | European Soil Database                              |
| <b>ET</b>                      | Evapotranspiration                                  |
| <b>EU-DEM</b>                  | European Digital Elevation Model                    |
| <b>FI</b>                      | Full irrigation                                     |
| <b><math>f_{max}</math></b>    | Maximum fractional saturated area                   |
| <b><math>f_{thresh}</math></b> | Tuning parameter in the CLM5 irrigation routine     |
| <b>G</b>                       | Soil heat flux                                      |
| <b>GDD</b>                     | Growing degree days                                 |
| <b>GDP</b>                     | Gross domestic product                              |
| <b>GPP</b>                     | Gross primary productivity                          |
| <b>H</b>                       | Sensible heat                                       |
| <b>IAC</b>                     | Institute of Atmospheric and Climate Science        |
| <b>IAV</b>                     | Inter-annual variability                            |
| <b>ICOS</b>                    | Integrated Carbon Observation System                |



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|                                   |   |
|-----------------------------------|---|
| <b>ICOS-bkp</b>                   | Backup ICOS climate station Selhausen                       |
| <b>IR</b>                         | Infrared  |
| <b>LAI</b>                        | Leaf area index   |
| <b>LE</b>                         | Latent heat   |
| <b>LPJmL</b>                      | Lund-Potsdam-Jena managed Land                              |
| <b>LSM</b>                        | Land surface model  |
| <b>LW<sub>in</sub></b>            | Incoming longwave radiation                                 |
| <b>MAE</b>                        | Mean absolute error   |
| <b>MBE</b>                        | Mean bias error   |
| <b>N</b>                          | Nitrogen  |
| <b>NEE</b>                        | Net ecosystem exchange                                      |
| <b>NPP</b>                        | Net primary productivity                                    |
| <b>PE</b>                         | Parameter effect  |
| <b>PFT</b>                        | Plant functional type                                       |
| <b>PHO</b>                        | Pinios Hydrologic Observatory                               |
| <b>r</b>                          | Pearson's coefficient of correlation                        |
| <b>R<sup>2</sup></b>              | Coefficient of determination                                |
| <b>R<sub>a</sub></b>              | Autotrophic respiration                                     |
| <b>R<sub>eco</sub></b>            | Ecosystem respiration                                       |
| <b>R<sub>h</sub></b>              | Heterotrophic respiration                                   |
| <b>RMSE</b>                       | Root mean square error                                      |
| <b>R<sub>n</sub></b>              | Net radiation   |
| <b>R<sub>s</sub></b>              | Soil respiration  |
| <b>SM</b>                         | Soil moisture   |
| <b>SMP</b>                        | Soil matric potential                                       |
| <b>TAHMO</b>                      | Trans-African Hydro-Meteorological Observatory              |
| <b>TERENO</b>                     | TERrestrial ENvironmental Observatories                     |
| <b>WMO</b>                        | World Meteorological Organization                           |
| <b>WSN</b>                        | Wireless sensor network                                     |
| <b><math>\psi_{target}</math></b> | Target soil matric potential in the CLM5 irrigation routine |



# 1 Introduction

Agriculture has been and continues to be an essential component of human development, shaping our societies and sustaining the world's population. Although the global share of employment in agriculture, forestry, and fishing has been declining in recent years, it remains the second largest source of employment and currently provides roughly a quarter of the world's population with livelihood [FAO, 2022]. The agricultural sector currently accounts for 4.3% of the global gross domestic product (GDP) and for as much as 25% of GDP in low-income countries [World Bank, 2021]. As such, it is crucial to economic development and poverty reduction.

Practicing agriculture involves transforming the world's landscapes and utilizing natural resources to meet human needs. Agricultural land use has been expanding due to population growth, economic development, and advancements in technology. Simultaneously, crop breeding and the widespread use of fertilizers and pesticides have boosted agricultural productivity since the green revolution in the mid-20<sup>th</sup> century [Perkins, 1990]. As a result, croplands and pastures now are the largest land use worldwide and occupy 37% of the global land surface (excluding Antarctica and inland waters) [FAO, 2021b].

The growing demand for food and the expansion of agricultural land made it imperative to increase agricultural production in regions with insufficient or irregular rainfall. This led to significant increases and modernization of irrigation infrastructure, especially during the green revolution [Angelakis et al., 2020]. Irrigation is the process of artificially applying water to the soil to meet crop water requirements, thereby enabling or enhancing crop growth and yield. While most of the cropland continues to be rainfed, the importance of irrigated agriculture in terms of food security is ever growing. According to the FAO [2022], the global land area equipped for irrigation increased by 20% since 2000 and has more than doubled compared to the 1960s. Currently, ~40% of global food supply is produced on irrigated land, which covers one fifth of the total agricultural area [WWAP, 2019]. Irrigation, especially for crop production, accounts for 70% of total freshwater

withdrawals worldwide, making it the largest freshwater consumer [Campbell *et al.*, 2017].

Despite the apparent societal benefits of providing livelihood and supplying food, modern agriculture has profound and often negative impacts on the natural environment. Local and regional farming practices can lead to odour and sound pollution, contamination of soil and water bodies through the percolation or runoff of fertilizers and pesticides, or soil degradation through soil erosion processes [Payraudeau and van der Werf, 2005]. Other effects act on a global scale such as land use and -cover change, emission of greenhouse gases and biodiversity loss [Ramankutty *et al.*, 2018].

Irrigation practices also show strong environmental effects across scales, profoundly affecting the water cycle, surface energy budget, and climate [Cook *et al.*, 2015]. Irrigation directly influences soil water content through the addition of water from other sources, e.g. groundwater or surface water, which affects hydrological processes such as deep percolation and runoff. Intensive irrigation generally reduces river flows and drives groundwater depletion [Thomas and Famiglietti, 2019], thus exacerbating water scarcity with consequent risks to natural ecosystems. At the same time, more water is introduced into the atmosphere by evaporation from the soil and through crops that readily transpire the water supplied through irrigation practices, thereby impacting the climate [Chen and Dirmeyer, 2020]. These feedbacks can be observed in regard to temperature, humidity, and precipitation [Cook *et al.*, 2015; Rappin *et al.*, 2022]. Studies showed effects such as cooling of summer temperatures [Chen and Dirmeyer, 2020; Lawston *et al.*, 2020; Lobell *et al.*, 2008a; Sacks *et al.*, 2009], increases or changes in precipitation amount and location [DeAngelis *et al.*, 2010; Devanand *et al.*, 2019; Tuinenburg *et al.*, 2011; Yang *et al.*, 2019], and increased atmospheric moisture [Xu *et al.*, 2019] over various irrigated areas.

Apart from the environmental impact, poor management of irrigation can also negatively affect crop production and increase water use conflicts. Over-irrigation can lead to leaching of fertilizers and pesticides and increased risk for plant disease [Irmak, 2008; Maharjan *et al.*, 2014]. Moreover, the use of poor irrigation water quality can cause soil salinity problems [Khan *et al.*, 2006; Zanchi and Cecchi, 2010]. All of the above can limit crop growth with negative effects on crop yield. Excessive or inefficient irrigation can result in high conveyance or application water losses leading to poor crop water use efficiency (CWUE), referring to the amount of yield produced per unit volume of water

consumed, and potentially leaving insufficient water available to crops later in the season [Akhtar *et al.*, 2018]. This can also affect other water users downstream of the river network or as shared groundwater body. Indeed, this has caused national and international conflicts in the past, especially in semi-arid and arid regions [Carkoglu and Eder, 2001; Houdret, 2012; Pacific Institute, 2022; Wiebe, 2001].

The current issues of today's agriculture are numerous and will be exacerbated by continuing climate change. In the coming years, securing and sustaining freshwater availability for human activities and natural ecosystems will be one of our major challenges [IPCC, 2022]. Global water availability is projected to decrease, especially in regions already suffering from severe water scarcity i.e., South and East Asia, the Middle East, Mexico, the western US, and the Mediterranean [Van Vliet *et al.*, 2021]. This is driven by decreases in water quantity, that is the availability of surface and groundwater resources, and water quality, such as salinity levels, both of which constrain irrigation [Van Vliet *et al.*, 2021]. At the same time, global agricultural production will have to keep up with the needs of a growing population. Global food demand is projected to rise by up to 62% between 2010 and 2050 [Van Dijk *et al.*, 2021]. Consequently, water consumption for agriculture, including rainfed and irrigated production, is expected to increase by about 19% by 2050 [WWAP, 2012].

Irrigated agriculture will continue to play a key role in sustaining and increasing agricultural production in the future. At the same time, it needs to reconcile the conflicting trends in water availability and water use, and deal with the numerous present and future challenges as elaborated above. A sound understanding of the effects of irrigation is required to derive effective adaptation and mitigation measures. This is not only necessary to avoid the further depletion of water resources and detrimental impacts on aquatic and terrestrial ecosystems but also to sustain a high level of crop production [Rosa, 2022]. To accomplish this goal, there is a need to improve agricultural water management across spatial and temporal scales, ranging from individual agricultural fields and growing seasons to large catchments and long-term trends.

To improve irrigation management, information about the conditions in the irrigated area must be available through measurements and monitoring. This information can subsequently be used to directly guide irrigation decisions in the field [Gu *et al.*, 2020; Hedley *et al.*, 2012] and evaluate the performance of existing irrigation systems [Akhtar

*et al.*, 2018] but also to better understand irrigation-climate interactions and inform modelling [*McDermid et al.*, 2023]. Unfortunately, irrigation practices are scarcely monitored and observations of irrigation, along with ancillary data such as meteorological data, soil moisture (SM), and other environmental variables are rarely available [*Dari et al.*, 2023; *Lawston et al.*, 2017; *Rappin et al.*, 2022].

Secondly, observations must be combined with the appropriate predictive tools, such as numerical models. These models should represent the agricultural system in interaction with other Earth-system processes to holistically study and understand irrigation impacts on crop growth and yield as well as on the surrounding environment, and to aid decision-making processes. This means that on one hand they need to provide an accurate representation of multiple crops and management options while, on the other hand, they should include aspects from a broader environmental context, for instance the impact of irrigation on regional climate or groundwater availability. Therefore, interactions and feedback mechanisms between land, water, and atmosphere including the hydrological and biogeochemical cycles within the Earth system must be captured [*Betts*, 2005; *Stehfest et al.*, 2007]. Current models are however associated with uncertainties and biases due to complex parameterizations, challenging physical representations, and spatial resolution [*Chen and Dirmeyer*, 2020; *de Vrese and Hagemann*, 2018; *Kueppers et al.*, 2008]. These aspects can lead to large errors in the estimation of irrigation water consumption or withdrawal, making it difficult to derive reliable recommendations for water resources management [*Felfelani et al.*, 2021; *Leng et al.*, 2017; *Pokhrel et al.*, 2015; *Zhang et al.*, 2020].

In essence, embracing a well-developed data and model-driven approach in irrigated agriculture can help to capitalize on the benefits irrigation is providing. At the same time, it has the potential to equip policymakers to take informed decisions for a better irrigation and water resources management. Ultimately, this can ensure economic viability and global food security, and improve environmental sustainability in the face of a changing climate.

## **1.1 Environmental data for irrigation and water resources management**

### **1.1.1 Understanding the importance of environmental data**

Access to comprehensive environmental data from different sources is paramount for agricultural and water resources management. Analysing this data can provide critical insights into the complex interplay between meteorological conditions, soil characteristics, and crop requirements. In this way, they are essential for decision-making and to develop, evaluate, and run models that simulate agricultural systems.

Among the most important environmental data are meteorological parameters such as air temperature, humidity, solar radiation, and precipitation. Meteorological parameters play a key role in determining plant growth, water requirements, and crop yields. Precipitation is a key factor in rainfed crop production, as it provides the water input without which crops cannot thrive. Air temperature and radiation influence the rate of photosynthesis which is directly linked to plant growth and yield [Hall and Rao, 1999]. Evapotranspiration (ET), a key parameter to define plant water requirements, is largely controlled by the presence of moisture in the air, which in turn is influenced by temperature, solar radiation, and wind speed [Jensen, 1968]. Moreover, meteorological data is one of the most important input data to initiate and run models used for agricultural applications [Venäläinen and Heikinheimo, 2002]. This requires precise and reliable measurements.

Furthermore, soil water is tightly linked to crop growth and irrigation management. It refers to the quantity of water within the upper layers of the soil that directly interacts with the atmosphere via ET, infiltration, and runoff [De Lannoy et al., 2019]. The water content in the root zone must be maintained at a level that ensures optimal transpiration to realize the full yield potential of the crop. Soil water status can be expressed as SM content, indicating the amount of water present in the soil, or soil matric potential (SMP), which expresses the relative availability of the soil water for plant uptake. Both variables are commonly used in irrigation scheduling [Blonquist Jr et al., 2006; Dukes et al., 2007; Gu et al., 2020; Millán et al., 2019; Miller et al., 2014; Zotarelli et al., 2011] but are also valuable for model evaluation and improvement [Devia et al., 2015; Vereecken et al., 2008; Zehe et al., 2005].

In addition, crop and agricultural management data are important factors influencing crop yield. These include crop-specific information such as crop phenology, leaf area index (LAI), and transpiration as well as data related to irrigation practices such as water withdrawal and quality, irrigation schedules and techniques, and other management information like fertilization or harvest practices [Deryng *et al.*, 2011; Licker *et al.*, 2010].

All of the above parameters can be highly variable in time and space. Meteorological phenomena for instance range from local microclimates over mesoscale events such as thunderstorms to global climate variations [Steyn *et al.*, 1981; Tavakolifar *et al.*, 2017]. Likewise, SM displays high spatial and temporal variability with a nonlinear effect on many environmental processes [Vereecken *et al.*, 2008; Western *et al.*, 2002]. Consequently, data acquisition must be tailored to different temporal and spatial scales depending on the application.

### **1.1.2 Scales of environmental data collection**

Advancements in instrumentation and digital technology have diversified the possibilities for data acquisition across multiple scales [NSF, 2007]. These methods encompass a range of techniques, from satellite-based remote sensing to ground-based in-situ measurements (Figure 1.1).

At a large regional to global scale, environmental data can be gathered through a variety of space- and airborne remote sensing techniques. For instance, remote sensing, combined with subsequent downscaling techniques, is used to estimate rainfall. Rainfall products are available at spatial resolutions between 1 and ~27 km and temporal resolutions ranging from half hourly to weekly [Kumar and Reshmidevi, 2013; Michaelides, 2019]. Similarly, land surface temperature can be obtained starting from ~1 km resolution even though its correlation to air temperature is a topic of ongoing research [Tomlinson *et al.*, 2011]. Global meteorological datasets are usually based on a combination of satellite and ground station data with reanalyses (hybrid model-observational data sets) or numerical climate modelling, and interpolated to resolutions of 0.1° and coarser [Davy and Kusch, 2021; Jiang *et al.*, 2018; Overpeck *et al.*, 2011]. Comparisons of some currently available datasets showed large differences in magnitude and variability of the estimated variables [Sun *et al.*, 2018].

For SM retrieval, satellite-based optical, thermal infrared, and microwave sensors are being used [Babaeian *et al.*, 2019]. The spatial resolution of the resulting products is



typically coarse, in the range of 25 and 50 km, while the temporal resolution ranges from daily to weekly [Brocca *et al.*, 2017] [Peng *et al.*, 2021]. Currently, some satellite missions aim to retrieve SM at 0.1 to 1 km spatial resolution at the regional to continental scale [Babaeian *et al.*, 2019; Mungen *et al.*, 2021]. Additionally, unmanned aerial vehicles equipped with sensors deliver measurements of airborne SM at higher spatial resolution (1-100 m) but at the expense of spatial extent and temporal coverage as they are typically flown over specific regions for a limited time only [Kumar and Reshmidevi, 2013].

The above techniques are based on an indirect linkage of the measured signal to SM and suffer from interference with clouds and vegetation resulting in relatively low accuracy when compared to ground based reference data [Gruber *et al.*, 2020]. Additionally, they usually yield information on near-surface SM (up to ~5 cm soil depth), which is insufficient for many agricultural applications that rely on root zone SM [Montzka *et al.*, 2017]. Other remote sensing products include estimates of crop ET or vegetation greenness (normalized difference vegetation index), crop classification or the mapping of irrigated areas. Despite their great potential, they are often limited in the amount of distinguished crop types and spatial coverage, and come with relatively high uncertainties [He *et al.*, 2023; Portmann *et al.*, 2010]. Although remote sensing products can deliver spatially continuous information over large areas, their limitations become apparent when addressing microscale variability. Downscaling or interpolation techniques are frequently used to infer regional or local information from these global data sets, which can be associated with great uncertainty and low skill in reproducing local conditions [Maurer and Hidalgo, 2008; Schoof, 2013]. Hence, ground-based measurements remain indispensable for investigating individual fields and small catchments due to the high spatial and temporal heterogeneity of e.g. meteorological variables and SM.

Locally, meteorological data can be obtained from the nearest ground-based weather station. These often belong to networks run by national meteorological services or research infrastructures. Such networks are typically well developed in high-income countries, but station coverage is often limited in rural areas, difficult terrain, or lower income countries requiring additional non-conventional stations to better observe the local climate [Mendelsohn *et al.*, 2007; Nsabagwa *et al.*, 2019; WMO, 2016].

For SM measurements, various techniques are available at the field or intermediate scale. These include non- or minimally invasive techniques such as electromagnetic induction [Sheets and Hendrickx, 1995] and electrical resistivity tomography [Brunet *et al.*, 2010] or emerging techniques such as cosmic ray neutron sensing [Zreda *et al.*, 2008] among others. The accurate determination of SM from the received signal can however be quite complex and sensitive to soil and vegetation properties [Brogi *et al.*, 2019; Brunet *et al.*, 2010; Jakobi *et al.*, 2018]. Also, the investigated soil depth can be limited and thus not represent the entire root zone depending on SM conditions [Köhli *et al.*, 2015] or on the measurement methodology [Bernard, 2003; Koyama *et al.*, 2017]. At the point-scale, in-situ sensors based on different electromagnetic principles are used to continuously measure SM [Bogena *et al.*, 2017]. In order to obtain representative measurements for a given area, a large number of in-situ sensors must be installed in multiple locations and at different depths within the soil profile [Bogena *et al.*, 2010]. However, applying such a high number of sensors requires cost effectiveness and automated solutions.

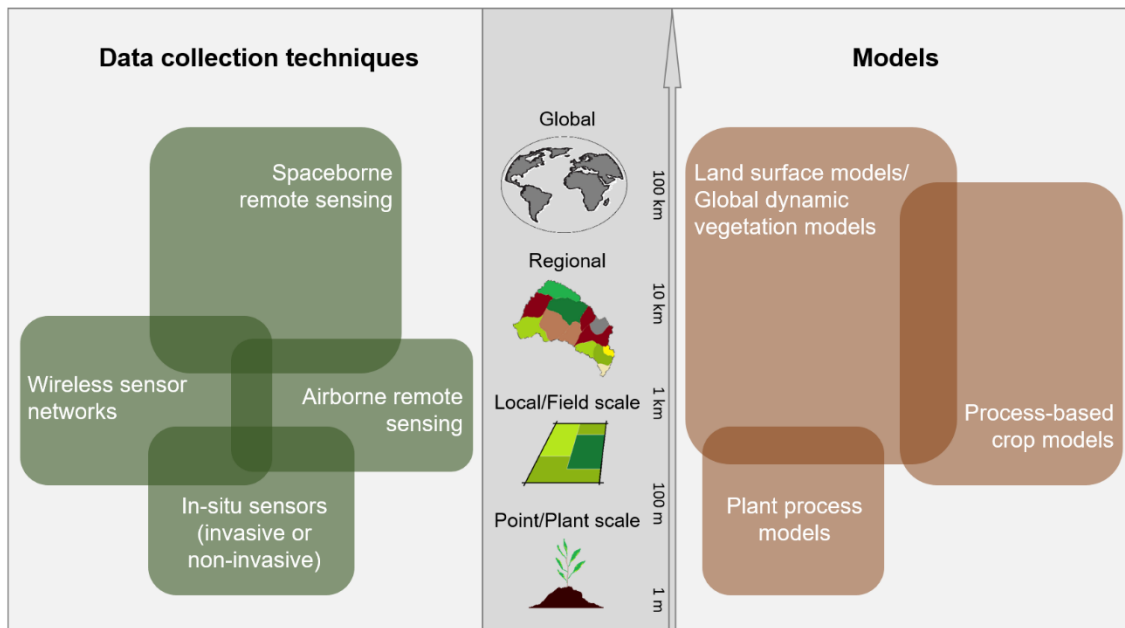


Figure 1.1 Typical spatial scales for the measurement and modelling of agricultural systems.

### 1.1.3 Low-cost sensors for wireless sensor networks

The rising demand for automated measurement systems has led to a range of low-cost sensors available from various manufacturers. Furthermore, recent advancements in electronics and communication technology have facilitated the integration of these sensors into wireless sensor networks (WSNs) for continuous environmental monitoring [Martinez *et al.*, 2004]. In WSNs, individual sensing devices communicate with one or

multiple base stations from where data is forwarded to a central server with remote access via a communication protocol [Hart and Martinez, 2006]. Commonly used protocols include ZigBee, Long Range (LoRa), and Narrow Band Internet of Things (NB-IoT). They make use of the low-power wide-area technology that enables wireless communication at relatively low cost and power consumption [Bogena et al., 2022].

To gather meteorological variables, low-cost all-in-one weather stations have recently gained popularity. They offer a compact and easy way to collect meteorological data at a given location. Due to their ease of use and cost efficiency, they are becoming widely used for field-scale applications [de la Concepcion et al., 2015; Tenzin et al., 2017; Watthanawisuth et al., 2009] and larger monitoring networks [van de Giesen et al., 2014]. For SM measurements, one type of suitable sensor is based on the capacitance method [Blonquist Jr et al., 2005], whereby the soil is incorporated as dielectric medium and the resultant output voltage is related to SM content [Bogena et al., 2007]. Other commonly used sensors are time domain reflectometry probes that determine the dielectric constant by wave propagation transmitted by two parallel metal probes [Tilse et al., 2023]. For SMP measurements, tensiometers are common though they are generally unsuitable for agricultural studies when crops grow under water-limited conditions. Instead, wettable porous media such as gypsum with embedded electrodes can be used for these applications [Brogi et al., 2022].

With the widespread use of low-cost sensors, concerns regarding their accuracy, reliability, and performance have been raised. These must be addressed as there can be trade-offs between low-cost and traditional sensors with the former potentially being less precise and less sensitive to the variable of interest [Okafor et al., 2020; Rai et al., 2017; Schwamback et al., 2023]. Hence, proper testing and calibration is indispensable to ensure suitability of these sensors for different applications, and to determine the factors that influence data quality for a given measurement [Bogena et al., 2017; Ioannou et al., 2021; Nsabagwa et al., 2019; Okafor et al., 2020]. If reliable, low-cost sensors in combination with WSNs offer diverse opportunities for data collection and monitoring at high spatiotemporal resolution complementary to more traditional monitoring and existing datasets.

### 1.1.4 Applications of wireless sensor networks

WSNs have found diverse applications across various fields and aspects of agricultural and water resources management and monitoring. Nowadays, they are widely used to directly support farmers in various management decisions. This recent data driven approach is called smart farming and is seen as a key component for sustainable agricultural management [Bach and Mauser, 2018; Lytos et al., 2020]. It aims to increase resource efficiency through precise input application, optimize yield, and generate high-resolution data to guide decision-making processes [Dhanaraju et al., 2022; Walter et al., 2017].

Due to its crucial role in modern agriculture, especially in arid and semi-arid regions, irrigation water management has become one of the main areas of application in smart farming. Different smart irrigation practices are explored to achieve more efficient and sustainable water use [Moysiadis et al., 2021; Touil et al., 2022]. Additionally, more effective irrigation systems like the use of drip and micro-irrigation, whereby water is delivered more directly to the plant root zone, have become more widespread [Hla and Scherer, 2003]. These systems minimize water loss due to evaporation and runoff, increase CWUE and improve crop yield [Obaideen et al., 2022]. Traditional irrigation practices, based on farmer experience and standard schedules are increasingly being replaced by automated irrigation systems. These systems integrate real-time data from various sources to remotely control, monitor, and adjust irrigation timing, duration, and intensity. These decisions are based on a variety of approaches from simple irrigation triggers (e.g., lower limit or threshold of SM or SMP), to regression algorithms and various machine-learning techniques, to more complex physically-based models [Gu et al., 2020].

Despite the benefits of smart farming, the high cost and advanced knowledge and skill needed to make proper use of such technologies pose a significant challenge for many small-scale farmers, especially in low-income countries [Walter et al., 2017]. To extend the focus beyond the scale of individual fields and single crop growing seasons, the installed WSNs can be integrated into a larger monitoring network. This is necessary as water management decisions are often taken at regional or catchment scale and need to be informed by an accurate understanding of the interacting processes occurring at this scale over time [Jensen and Illangasekare, 2011].

Recognizing this necessity has led to the establishment of hydrological observatories that intend to cover whole catchments with a dense observational network. One aim of these observatories is to collect long-term hydrological measurements to predict the consequences of climate and land use changes, and to take a holistic approach to water resources management [Bogena *et al.*, 2018; Jensen and Illangasekare, 2011]. Several of such observatories across the world investigate the impact of agricultural systems on the environment. The Hyderabad Observatory in India for instance looks at various components of the water cycle in intensely irrigated areas [Maréchal *et al.*, 2018]. The Northeast German Lowland Observatory as part of the German TERrestrial ENVironmental Observatories network (TERENO) includes several intensely managed agricultural sites [Heinrich *et al.*, 2018] and the Dutch Hupsel Brook catchment was established with the aim to improve agricultural water management [Brauer *et al.*, 2018]. Observatories with a focus on the Mediterranean area were established in France and Tunisia [Molénat *et al.*, 2018], Italy [Romano *et al.*, 2018], and Greece [Pisinaras *et al.*, 2018] and put an emphasis on sustainable water management among others.

Notably, the importance of environmental data to further improve agricultural and water resources management cannot be overstated. Low-cost sensors in combination with WSNs offer new opportunities to increase data availability and to better capture the heterogeneity and spatiotemporal variability of e.g. SM across larger areas [Vereecken *et al.*, 2019]. The sensors, though cost-effective, should however undergo rigorous testing and calibration to address data quality concerns and make them suitable for various applications. If leveraged correctly, WSNs integrated into hydrological observatories can greatly contribute to not only providing a holistic understanding of local and regional scale processes relevant for irrigation and water resources management but also to developing, calibrating and validating various models used in this context.

## 1.2 Modelling agricultural systems

Modelling is an essential tool not only for farm-scale crop yield prediction and irrigation management but also to guide decision-making at regional or catchment scale and beyond for improved agricultural and water resources management. A multitude of models is available for the simulation of agricultural systems at different scales (Figure 1.1). These models can vary greatly in their degree of process representation, physical basis, and input requirements.

### 1.2.1 Crop modelling approaches

Generally, crop modelling can be used to simulate crop growth and yield in agricultural systems. Available approaches include empirical or process-based models that were developed for field-scale applications or for global dynamic vegetation and land-surface modelling [Elliott *et al.*, 2015; White *et al.*, 2011]. Empirical or statistical models estimate climate-yield relationships based on observed datasets of yield and climate variables, and are mainly applied for agricultural climate impact assessments [Gornott and Wechsung, 2015; Lobell *et al.*, 2008b]. However, as their equations are solely fitted based on available observations, they do not explain the underlying mechanisms of yield variation and have limited applicability under climatic or environmental conditions beyond the observed ones [Holzkämper, 2017].

Other models are based on a mechanistic understanding of biophysical processes and therefore provide a good basis to assess management or climate change impacts on crops and their interactions in different agroecosystems [Kephe *et al.*, 2021]. Certain models represent specific biophysical processes such as photosynthesis [Farquhar *et al.*, 1980; Wang *et al.*, 2014], respiration [Sweetlove *et al.*, 2013], or crop growth and development [Prusinkiewicz and Runions, 2012]. They typically operate at narrow spatiotemporal scales to assess how a process is affected by environmental parameters for a particular crop type [Marshall-Colon *et al.*, 2017].

Beyond individual processes or plants, dynamic process-based crop models (CMs) were developed to simulate crop development and yield in relation to environmental conditions (e.g., SM, air temperature, CO<sub>2</sub> concentration) and management practices (e.g., irrigation, nitrogen fertilization) at the field scale [Muller and Martre, 2019]. Compared to empirical models, they require a larger amount of input data (e.g. soil and crop parameters) due to

their greater complexity [*Manivasagam and Rozenstein, 2020*]. Some of the early, widely known CMs are the CERES model for maize [*Jones et al., 1986*] and wheat [*Ritchie and Otter, 1985*], SUCROS for spring wheat [*Van Laar et al., 1997*], and SOYGRO for soybeans [*Wilkerson et al., 1983*].

The above mentioned CMs were later incorporated into the decision support system for agrotechnology transfer (DSSAT) for better compatibility and application [*Jones et al., 2003*]. This suite of CMs currently includes models for various annual crops e.g. grains, legumes, and vegetables as well as perennial forage crops [*Pereira et al., 2020*]. DSSAT can be used to simulate crop growth, development, and yield and to investigate crop management decisions over single or multiple seasons under the consideration of soil, crop phenotype, and weather [*Jones et al., 2003*]. Other widely used multi-crop models include EPIC [*Williams et al., 1989*], CropSyst [*Stöckle et al., 2003*], AquaCrop [*Steduto et al., 2009*], or the APSIM suite of CMs [*Keating et al., 2003*] and can simulate a variety of annual and perennial crops and management options similarly to DSSAT. Apart from biophysical processes, APSIM can also simulate economic and ecological outcomes of specific crop management practices under changing climatic conditions [*Keating et al., 2003*].

The models differ in terms of complexity, i.e. AquaCrop focusses on simulating the effect of water limitation on potential crop yield while the DSSAT model family integrates crop responses to soil water, nutrients, and soil carbon (C). EPIC and CropSyst additionally integrate climate and management effects on soil erosion while APSIM is more detailed in representing crop growth processes and differentiates between individual plant components [*Holzkämper, 2017*].

Most CMs were designed for field-scale simulations with one exception being the regional-scale crop model GLAM [*Challinor et al., 2004*], but are often applied at regional or even global scale [*Challinor et al., 2018; Holzkämper, 2017*]. This however can lead to computational challenges and may impact their ability to accurately represent the spatial heterogeneity of climate variability on yield [*Doering and Otto, 2002*]. Additionally, because of their development as standalone CMs, they typically lack a more detailed description of the soil profile including soil hydraulic properties that are key to adequately simulate soil water status and irrigation requirements [*Vereecken et al., 2016*]. Other approaches therefore combine CMs with transient state models, e.g. the crop

growth model WOFOST and the hydrologic model HYDRUS-1D [Zhou *et al.*, 2012] or the agro-hydrological model SWAP and the crop growth model EPIC [Xu *et al.*, 2013] to improve the representation of water dynamics in the soil. Moreover, CMs neglect the wider interactions of crop and environment [Levis *et al.*, 2012]. For instance, climate change will affect water resources with consequent impact on water availability for irrigation [Arnell, 1999; Döll, 2002].

As croplands cover substantial areas of land and greatly impact the Earth system, there has been increasing interest and need to model these interactions of crop production and management with local climate, hydrology, and land surface processes. This has led to the inclusion of agricultural systems into spatially distributed models with broader scopes such as dynamic global vegetation models, e.g. the Lund-Potsdam-Jena managed Land model (LPJmL) [Bondeau *et al.*, 2007], river basin models such as SWAT/SWIM [Arnold *et al.*, 1998; Krysanova *et al.*, 2000], or different land surface models (LSMs) [Fisher and Koven, 2020] that can be coupled to climate models and are typically used for regional to global scale modelling. Due to their large-scale application and their origin from other disciplines (e.g. hydrology, terrestrial ecosystem or climate sciences), crop and management representations in these models are often comparatively simpler than those of field-scale CMs [Holzkämper, 2017; Manivasagam and Rozenstein, 2020]. However, LSMs represent hydrology, surface energy balance, and biogeochemical cycles and could thus appear more suitable to evaluate the environmental impacts of agriculture in the Earth system in a more holistic way [Blyth *et al.*, 2021; Peng *et al.*, 2020].

### **1.2.2 Land surface models**

LSMs form the land component of earth system models and depict all terrestrial ecosystem processes. They require meteorological, land cover, and soil data to simulate the interactions between land, vegetation, water, and the atmosphere at large regional, continental, or global scales [Bonan, 2019]. LSMs originated from the climate modelling community where their primary purpose was to deliver the physical boundary conditions at the land-atmosphere interface to study the influence of land on weather and climate. However, the role of the terrestrial biosphere and land surface itself with the related biogeophysical and biogeochemical processes has since gained greater attention and has led to many further developments of LSMs across a broad range of spatial and temporal scales [Buechel, 2021; Fisher and Koven, 2020]. Their application has thus expanded to



a wide variety of contexts including the effects and potential risks of land use and change on climate, terrestrial and aquatic ecosystems as well as human societies [Blyth *et al.*, 2021; Fisher and Koven, 2020]. As a result, LSMs have greatly evolved in the representation of processes to include SM dynamics, land surface hydrological processes, C and nitrogen cycling, land cover, and human land management such as crop production [Lawrence *et al.*, 2019].

### 1.2.3 Crop representations in LSMs

Initially, crops were represented by a generic crop type similar to grasses in many LSMs [Lombardozzi *et al.*, 2020]. Various LSMs, such as ORCHIDEE, the Community Land Model (CLM), JULES and Noah-MP have since incorporated process-based CMs to dynamically model crops and crop management [Levis *et al.*, 2012; Liu *et al.*, 2016; Osborne *et al.*, 2014; Wu *et al.*, 2016]. Crop representations typically include a description of crop phenology, partitioning of dry matter, and management practices such as sowing, fertilization, and harvest. Similar to classical CMs, crop growth is governed by crop phenological phases that are triggered by growing degree-day thresholds [Liu *et al.*, 2016]. In CLM version 5 (CLM5), planting, leaf emergence, grain fill, and harvest are distinguished while other LSMs may use additional or fewer phenological phases. During the growing season, C and N are allocated based on C:N ratios of the individual plant organs (leaf, stem, fine roots, grain), whereby N is supplied by the soil mineral N pool. At harvest, the grain pool is transferred to a grain product pool and exported as yield [Lombardozzi *et al.*, 2020]. The integration of crops into LSMs has significantly improved the simulation of the seasonal evolution of LAI [Osborne *et al.*, 2014; Wu *et al.*, 2016], gross primary productivity [Drewniak *et al.*, 2013; Osborne *et al.*, 2014], net ecosystem exchange and latent heat [Levis *et al.*, 2012; Lokupitiya *et al.*, 2016].

However, the diversity of crop types, cultivars, and management practices is still greatly simplified in these models [Lombardozzi *et al.*, 2020]. This has resulted in inaccurate representations of phenology and crop yield [Chen *et al.*, 2018; Lombardozzi *et al.*, 2020; Sheng *et al.*, 2018]. Besides a limited number of major annual crop types (e.g., wheat, soy, corn, rice) descriptions of other crops such as perennials or less common grains or tuber crops are still scarce, partially due to a lack of comprehensive datasets to parameterize these crops. Recently, some efforts have been made to improve crop growth and management processes or to include additional crop types and cropping systems into

LSMs and other global modelling environments. For instance, *Peng et al.* [2018] developed a new maize model in CLM4.5 and *Boas et al.* [2021] implemented a subroutine for winter wheat and new parameters for sugar beet, potatoes, and winter wheat in CLM5. Bioenergy crops [*Schaphoff et al.*, 2018] and agricultural trees [*Fader et al.*, 2015] were included in the LPJmL model. Moreover, *Fan et al.* [2015] parameterized oil palms, as a perennial evergreen crop within CLM4.5 and *Cheng et al.* [2020] included two perennial grasses for energy production in CLM5. These extensions improved the simulation of crop phenology, yield, and the surface energy and C fluxes [*Boas et al.*, 2021; *Peng et al.*, 2018], and continue to increase the ability of LSMs to represent a greater diversity of agricultural systems.

### 1.2.4 Irrigation in LSMs

Irrigation has only recently been acknowledged as an important driver of Earth system processes to be included in LSMs. Consequently, irrigation is still largely underrepresented or implemented in a rather simplistic way in many LSMs [*McDermid et al.*, 2023; *Pokhrel et al.*, 2016].

*De Rosnay et al.* [2003] incorporated an irrigation scheme in ORCHIDEE to examine the regional impacts of irrigation on energy partitioning. In their study, daily irrigation requirements were calculated based on the difference between potential evaporation multiplied by a crop coefficient and precipitation. Actual irrigation was then determined depending on water availability in the river system and aquifer as simulated by a routing scheme. Other authors prescribed a fixed irrigation rate or implemented dynamic irrigation schemes based on defined SM thresholds in the root zone to trigger irrigation in JSBACH, NoahMP and CLM4 using satellite-derived data to identify irrigated areas [*de Vrese et al.*, 2016; *Levis and Sacks*, 2011; *Ozdogan et al.*, 2010; *Sacks et al.*, 2009]. Using this approach, irrigation is driven by soil water status independent of management techniques or water availability. Consequently, irrigation and irrigation-induced impacts simulated in these studies have shown various issues including overestimation of irrigation amounts and duration or runoff, and underestimation of the change in latent heat [*Kueppers and Snyder*, 2012; *Lawston et al.*, 2017; *Sacks et al.*, 2009].

More recently, model developments added new capabilities such as distinguishing different irrigation techniques (i.e. sprinkler, surface, drip irrigation) [*Leng et al.*, 2017; *Pokhrel et al.*, 2015; *Yao et al.*, 2022] or including different sources for irrigation water

withdrawal including groundwater pumping [Leng *et al.*, 2017; Xia *et al.*, 2022] in CLM5, NoahMP, ACME or HiGWMAT. Others added water regulation modules accounting for other water uses next to irrigation [Pokhrel *et al.*, 2012], and limitations on water availability [Yin *et al.*, 2020] to MATSIRO and ORCHIDEE, respectively. These developments improved the performance of the models when compared to observed river discharge, irrigation water withdrawals, and groundwater depletion. However, given the various approaches to model irrigation, simulated irrigation exhibits considerable discrepancies especially at local and regional scales [Haddeland *et al.*, 2014; McDermid *et al.*, 2023; Pokhrel *et al.*, 2016]. The coarse scales (10–100 km) at which the mentioned irrigation studies were performed and the lack of local irrigation data further contribute to these uncertainties [Lawston *et al.*, 2017; McDermid *et al.*, 2023]. As more irrigation data become available at higher resolution, they can be used to better evaluate and improve existing irrigation schemes. This can give further insight into the effects of irrigation and its current representations in LSMs down to the field scale [Huang *et al.*, 2022; Lawston *et al.*, 2017].

Clearly, efforts are ongoing to improve the simulation of human land and water management in terms of crop and irrigation representations in LSMs. While noteworthy progress has been made in both areas, this work needs to be continued to include missing crop types, e.g. perennial crops, and to more realistically represent local irrigation practices. This will allow to better account for regions with a more diverse agricultural landscape, e.g. mixed annual or perennial cropping systems.

## 1.3 The Mediterranean context

Although most of the work in this thesis aims to be applicable across the world, the focus is put on the Mediterranean. This region combines a rich history and biodiversity, a wide range of traditional and modern agricultural activities, a highly variable climate, different degrees of economic development, chronic water scarcity and high environmental vulnerability [Tramblay *et al.*, 2020]. All of these factors create a unique environment and necessity for research and policy development for sustainable irrigation practices and water resources management. Moreover, the lessons learned from this region can have a broader applicability and offer valuable insights to address challenges related to agriculture, water, and climate change globally.

### 1.3.1 Characteristics of the region

The Mediterranean region spans over southern Europe, Northern Africa, and the Middle East. Its climate falls in the transitional zone between the subtropical and temperate zones and is characterized by hot and dry summers and cool wet winter periods with high intra- and inter-annual variability in rainfall [Joffre and Rambal, 2001; Lionello *et al.*, 2006]. The region has a diverse geography and rich biodiversity with a large number of endemic plant species, while at the same time conditions in the area are suitable to grow a wide variety of crops [Myers *et al.*, 2000].

The Mediterranean has been a cradle of agriculture dating back millennia [Aguilera *et al.*, 2020]. Agricultural practices have shaped the landscape, cultural identity, and economic growth of the region. Until today, agricultural production is of high economic value employing more than a fifth of the population and contributing > 10% of GDP in some Mediterranean countries [CIHEAM, 2009]. Next to annual crops including cereals and pulses, the cultivation of perennial crops, like olive trees, vineyards, and various fruit and nut trees, is an integral part of the region's agricultural landscape. Farm sizes are generally small compared to other agricultural areas, which creates a fragmented, diverse landscape, and a challenge to farmers who often struggle to provide sufficient income to adequately support their families [Lobianco and Roberto, 2006]. Considering the semi-arid conditions and irregular rainfall patterns, irrigation has been a cornerstone of agriculture in the Mediterranean to achieve adequate crop growth and yield [Semple, 1929]. As a result, irrigated land has been expanding continuously, facilitating food production and securing livelihoods for a growing population [Daccache *et al.*, 2014].

Presently, irrigated agriculture is responsible for around 50% of total water withdrawal, with strong sub-regional differences ranging from 11% in Croatia and France to > 80% in Egypt, Greece, and Syria [FAO, 2022].

### **1.3.2 Environmental pressures**

The Mediterranean region faces mounting pressure on its water resources due to the dependence on irrigation combined with other factors including rapid population growth, urbanization, and climate change [Fader *et al.*, 2016]. Together with poor water governance and inefficient irrigation practices, this has repeatedly led to over extraction of water, decline of groundwater quality, soil degradation, and environmental pollution [Aureli *et al.*, 2008; Daccache *et al.*, 2014; Kurunc *et al.*, 2016; Pisinaras *et al.*, 2010]. Additionally, the Mediterranean has been declared one of the climate change hotspots and is likely to experience more frequent and intense heat waves and prolonged periods of drought [Diffenbaugh and Giorgi, 2012; IPCC, 2012]. Consequently, certain areas could see up to 40% decrease in winter precipitation under RCP8.5 scenario (the Representative Concentration Pathway that would lead to 4 °C of global warming) [Tuel and Eltahir, 2020].

The effects of climate change on Mediterranean agriculture are manifold. Higher temperatures together with changes in the amount and distribution of rainfall will result in increased competition for the already limited water supplies in many Mediterranean countries [Cramer *et al.*, 2018; Iglesias and Garrote, 2015; IPCC, 2022; Tuel and Eltahir, 2020]. Additionally, yield reduction and increased crop water demand are expected for various spring-grown crops. While the increases in CO<sub>2</sub> may reduce these negative effects partially, the yield loss will hardly be recovered entirely [Skuras and Psaltopoulos, 2012]. The changes in temperature and precipitation might render some crops unsuitable for production in the Mediterranean [Ceglar *et al.*, 2019; Zagaria *et al.*, 2023]. Moreover, crop phenological development will likely shift to earlier in the year which can result in yield decline for certain crops [Moriondo and Bindi, 2007; Zagaria *et al.*, 2023]. Furthermore, irrigation water requirements will be strongly affected, for example, the southern and eastern Mediterranean is expected to see an increase of up to 35% [Fader *et al.*, 2016].

### 1.3.3 Need for adaptation measures

Water scarcity, poor irrigation management, and progressing climate change have raised concerns about the sustainability and resilience of Mediterranean agriculture and have emphasized the need for adaptation measures [Fader *et al.*, 2016]. These measures include the switch to more efficient irrigation systems, adjustment of irrigation schedules, diversification of water resources, storage and harvesting of rainwater, or water pricing [García-Tejero *et al.*, 2014; Harmanny and Malek, 2019]. In addition to measures focussed on alternative water resources and improved irrigation efficiency, crop selection and management can be effective measures to mitigate climate change impacts. The FAO, for instance, has emphasized the role of perennial agriculture in protecting and improving soil ecosystem health and enhancing food security [Batello *et al.*, 2014; Glover *et al.*, 2010].

Supporting sustainable agricultural and water resources management will require a holistic understanding of the state and potential developments of Mediterranean crop production and the role of irrigation in water resources. The high diversity and distinctive characteristics of Mediterranean agricultural systems pose a challenge to establishing a comprehensive data base as well as to the development of modelling tools that can accurately represent these systems. Modern data observation networks and cost effective sensors can help leverage data availability of e.g., weather, soil, crop, and irrigation, which unfortunately is often limited, especially in southern Mediterranean countries [Fader *et al.*, 2015]. In addition, the continued development of process representations in LSMs can equip these models to guide decisions in crop production, irrigation, and water resources management at different scales to secure environmental sustainability as well as economic viability of Mediterranean agriculture.

## 1.4 Research objectives and thesis outline

The overall aim of this thesis is to improve the representation of crops and irrigation in LSMs and combine them with local observational data to assess crop water requirements and derive management recommendations that can ultimately lead to reduced irrigation water consumption while sustaining agricultural yield in the context of the Mediterranean region. The following sub-objectives were defined to achieve this goal.

The first objective is to examine the use of low-cost weather sensors to deliver accurate data and improve overall data availability for field-scale crop and water management as well as regional agricultural, hydrologic, or climate research and modelling. These sensors should be robust, reliable, easy to use and maintain, and should not deviate strongly from high-end sensors in order to be adequate for use in single site monitoring or as components of larger environmental observatories.

The second sub-objective is to improve the representation of perennial crop types within LSMs by including deciduous fruit trees in CLM5. To achieve this, the current model descriptions of annual crops and natural vegetation must be expanded to include new features that are unique to fruit trees and orchards. This should result in more reliable simulations of crop growth and water requirements, and reduce the existing bias in the representation of the biogeophysical and biogeochemical processes in regions where this type of cultivation is prevalent.

The third sub-objective addresses the critical role of irrigation in global food production, especially in semi-arid regions, and its impact on yield, land surface processes, and water resources. Despite its critical importance, irrigation is not yet accurately accounted for in most LSMs. It is therefore necessary to assess and improve the existing model capabilities, demonstrate how these improvements are relevant in advancing the incorporation of human land-water management into global LSMs, and illustrate how they can contribute to more sustainable irrigation and water resources management.

To address these objectives, the thesis is structured into five parts. Chapter 1 provided a general introduction and background to the following three chapters that are based on two peer-reviewed and published papers and one submitted paper.

In Chapter 2, the performance of the ATMOS41 all-in-one weather station (METER Group Inc.) is evaluated and its potential use in the context of microclimate monitoring for various user applications as well as research activities is discussed. This cost-effective and easy-to-use station can increase the availability of data, especially in remote regions and low-income countries. However, adequate calibration and testing should be performed to ensure sufficiently high data quality. Under this objective, three ATMOS41 were installed next to a high-performance reference station at an experimental site in Germany. Meteorological data was collected over a three-month period at a 10-min interval. Collected data of solar radiation, precipitation, air temperature, relative humidity, atmospheric pressure, wind speed, and wind direction was analysed using graphical and statistical techniques. The inter-sensor variability between the three stations and the overall quality of the weather data from the ATMOS41 compared to the reference station was assessed. Moreover, systematic and random errors were determined and potential limitations for the deployment of the ATMOS41 were discussed.

In Chapter 3, CLM5-FruitTree, a new sub-model for perennial deciduous fruit trees, is presented, which improves the representation of agricultural systems within the LSM CLM5. The development encompassed (1) a new perennial crop phenology description, (2) an adapted C and nitrogen allocation scheme, considering both storage and photosynthetic growth of annual and perennial plant organs, (3) typical management practices associated with fruit orchards, and (4) the parameterization of an apple plant functional type (PFT). Extensive field measurements from an apple orchard in South Tyrol, Italy were available to develop and test the sub-model. Measurements of biomass and C and nitrogen ratios of the individual plant organs, root distribution as well as literature values were used to parameterize the apple PFT. Additionally, a simple one-by-one sensitivity analysis was performed to further tune model parameters and assess the influence of newly added parameters on the simulation results. Finally, the simulation results were compared to observed LAI, yield, C, energy, and water fluxes from an eddy covariance station, and SM measurements.

Chapter 4 focusses on the representation of irrigation in CLM5. The new CLM5-FruitTree sub-model, as presented in Chapter 3, was used to assess irrigation practices and water consumption in a small Greek catchment dominated by apple orchards. First, the representation of local irrigation practices and resulting SM dynamics and crop



growth was evaluated at the point-scale. An irrigation data stream was implemented that allows to directly read in measured irrigation data. The simulations were compared to data collected from WSNs in two highly instrumented apple orchards and were forced with atmospheric data obtained from two ATMOS41 weather stations evaluated in Chapter 2. Subsequently, a regional modelling case was set up to compute irrigation requirements for the entire catchment. Based on these modelling results and using the irrigation stream, different irrigation deficit scenarios were created and their effect on yield and CWUE was examined to derive recommendations for regional irrigation management.

Finally, the thesis concludes with Chapter 5, in which a synthesis of this work is provided and directions for future research and applications are discussed.



## 2 Performance of the ATMOS41 All-in-One Weather Station for Weather Monitoring

This chapter is based on the following journal article:

**Dombrowski, O.**, Hendricks Franssen, H. J., Brogi, C., & Bogena, H. R. (2021). Performance of the ATMOS41 All-in-One Weather Station for Weather Monitoring. *Sensors*, 21(3), 741. <https://doi.org/10.3390/s21030741>

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### **Abstract**

Affordable and accurate weather monitoring systems are essential in low-income and developing countries and, more recently, are needed in small-scale research such as precision agriculture and urban climate studies. A variety of low-cost solutions are available on the market, but the use of non-standard technologies raises concerns for data quality. Research-grade all-in-one weather stations could present a reliable, cost effective solution while being robust and easy to use. This study evaluates the performance of the commercially available ATMOS41 all-in-one weather station. Three stations were deployed next to a high-performance reference station over a three-month period. The ATMOS41 stations showed good performance compared to the reference, and close agreement among the three stations for most standard weather variables. However, measured atmospheric pressure showed uncertainties  $> 0.6$  hPa and solar radiation was underestimated by 3%, which could be corrected with a locally obtained linear regression function. Furthermore, precipitation measurements showed considerable variability, with observed differences of  $\pm 7.5\%$  compared to the reference gauge, which suggests relatively high susceptibility to wind-induced errors. Overall, the station is well suited for private user applications such as farming, while the use in research should consider the limitations of the station, especially regarding precise precipitation measurements.

## 2.1 Introduction

Weather monitoring plays a central role in the understanding of the hydrological cycle, weather forecasting, risk assessment and management as well as agricultural planning, the administration of natural resources, climate change studies and other public and private interests. Despite the fact that modern automatic weather station networks are typically well developed in high-income countries, data quality and station coverage are often limited in low-income countries due to high instrumentation and maintenance costs [Nsabagwa *et al.*, 2019; Pietrosevoli *et al.*, 2019; WMO, 2016]. Consequently, resources and trained personnel to set up and maintain a sufficient number of stations are lacking to adequately cover the spatiotemporal variability of meteorological variables [Sabatini, 2017; WMO, 2009]. Additionally, growing interest in microclimate monitoring for precision agriculture [de la Concepcion *et al.*, 2015; Tenzin *et al.*, 2017; Watthanawisuth *et al.*, 2009] or urban climate and heat island studies [Gaitani *et al.*, 2011; Tomlinson *et al.*, 2013] requires weather stations that are inexpensive, efficient, and provide local and reliable data for modelling applications. Ideally, the design of such weather stations meets the following criteria: (i) robustness to reduce calibration frequency; (ii) compact design for ease of handling and to minimize sensor damage; (iii) low maintenance; (iv) low power requirements; (v) low cost; (vi) compatibility with different logger systems; (vii) wireless communication.

With the increasing use of wireless sensor networks [Yick *et al.*, 2008], various non-standard low-cost weather monitoring systems have been developed in the past few years using a wide range of sensor hardware and different microcontroller architectures, such as Arduino [Katyal *et al.*, 2016; Lopez and Villaruz, 2015; Saini *et al.*, 2016] or Raspberry Pi [7,15,16]. These stations can be very cost effective, with prices of several hundred Euros [Pietrosevoli *et al.*, 2019], but they often lack adequate calibration and testing, raising concerns about the accuracy, precision, and reliability of the collected data [Gunawardena *et al.*, 2018]. However, information on data quality in terms of both the accuracy and repeatability of such low-cost weather stations is crucial for modelling applications and decision-making [Aponte-Roa *et al.*, 2018; Muller *et al.*, 2015]. Furthermore, designing these non-standard devices requires sufficient knowledge of the associated hardware and software for installation and maintenance, while the moving parts may be susceptible to failure. Commercial all-in-one weather stations, e.g., [Environmental XPRT, 2020; Gill Instruments Limited, 2023; Met One Instruments Inc.,

2023], that incorporate multiple sensors in a single unit can be a viable alternative as they are easily deployable, generally cheaper than standard weather stations composed of individual sensors, and include manufacturer reported accuracy, precision, and calibration details. On the downside, they are less flexible in terms of adding or exchanging sensors and may suffer from interference between sensors due to their compact architecture [Warne, 2017]. Nonetheless, their plug-and-play principle and the compact design are clear advantages since they facilitate non-expert use and make them suitable for continuous deployment in rural or remote areas.

This study focuses on the assessment of the ATMOS41 all-in-one weather station that holds 12 embedded sensors, developed and produced by METER Group, Inc. The station is currently used in sub-Saharan Africa to improve crop production of maize [Mutuku *et al.*, 2020] and to build the Trans-African Hydro-Meteorological Observatory (TAHMO) network [TAHMO, 2020]. TAHMO aims at installing 20,000 hydro-meteorological stations across sub-Saharan Africa and collected data will be used for educational purposes at local schools as well as aid in scientific modelling, early warning systems, and the analysis of water availability [van de Giesen *et al.*, 2014]. Furthermore, the ATMOS41 has recently found applications in crop research and private sector sensor networks of various industrialized countries. In Portugal, the station is being used in the development of a forest monitoring system for fire detection [Brito *et al.*, 2020] and in the field of smart agriculture to improve vineyard management practices [Valente *et al.*, 2020]. In addition, the ATMOS41 is part of the Montana Mesonet monitoring stations in the Upper Missouri River Basin, where collected data are used for drought detection and natural resource management, amongst others [Jencso *et al.*, 2019]. Further applications include the investigation of crop water stress in apple orchards at Washington State University [Mohamed *et al.*, 2019] and the estimation of the plant growth status of paddy rice in Japan [Xie *et al.*, 2020].

METER and partners provide reports of calibration and sensor performance tests for the complete weather station or for individual components performed in the lab or in outdoor testbeds of the METER Pullman campus [METER Group, 2018]. Furthermore, [Anand and Molnar, 2018] conducted a first-order performance analysis of the early version of the station. The study compared 6 months of data recorded in 2017/2018 by the ATMOS41 station against a weather station of the Institute of Atmospheric and Climate Science (IAC) of ETH Zurich and a SwissMetNet solar radiation station located at 2.5

km distance from the test site. Overall, the ATMOS41 showed similar performance to the IAC station, but the authors suggested that further tests are needed.

Since its first release in 2017, several improvements of the ATMOS41 station were developed, some of which directly affect the measurement of certain variables and the overall performance of the station [Ayman]. These changes include: (i) improved sensor geometry to avoid adverse effects on wind measurements caused by heavy rain, (ii) improved sensor firmware and wind sensing algorithm, (iii) upgraded sensors and the addition of a secondary calibration for relative humidity and atmospheric pressure.

Considering the wide use of the ATMOS41 weather station for small- and large-scale weather monitoring in sub-Saharan Africa [Mutuku *et al.*, 2020; TAHMO, 2020; van de Giesen *et al.*, 2014] as well as industrialized countries [Brito *et al.*, 2020; Jencso *et al.*, 2019; Mohamed *et al.*, 2019; Valente *et al.*, 2020; Xie *et al.*, 2020], independent testing under “out of the lab” conditions can provide further insight and eventually identify possible limitations of the ATMOS41 station. In this way, a thorough performance assessment can inform private costumers and research organizations regarding the potential fields of application and provide impulses for further hardware or software developments. Therefore, the aim of this study is to carry out such in-depth assessment through direct comparison to an independent, high-performance weather station as well as the inter-comparison of multiple ATMOS41 stations. Within this context, the following questions will be addressed:

- What is the quality of weather data from the ATMOS41 weather station?
- What systematic or random errors affect the ATMOS41 station?
- How well does the ATMOS41 station perform compared to a high precision, high quality weather station?
- What are the limitations of the ATMOS41 station?

## 2.2 Materials and Methods

### 2.2.1 ATMOS41 all-in-one weather station

The ATMOS41 is an all-in-one weather station developed by METER Group, Inc. (Pullman, WA, USA). The device is rather inexpensive for developed countries (below EUR 2000), has a compact design with no moving parts, and can be mounted with minimal effort to ensure easy deployment in a variety of terrains and locations. The station has 12 embedded sensors that measure standard weather variables, namely solar radiation, precipitation, air temperature, relative humidity, atmospheric pressure, wind speed and direction, plus additional parameters such as lightning strike count or compass heading. Further characteristics of the station are summarized in Table 2.1.

Table 2.1 Characteristics of the ATMOS41 all-in-one weather station.

| Characteristic         | ATMOS41   |
|------------------------|---|
| Manufacturer           | METER Group, Inc.   |
| Cost                   | EUR 1750  |
| Dimensions             | Height: 34 cm, $\varnothing = 10$ cm  |
| Warranty               | 1 year  |
| Installation           | Mount on pole, stand, or tripod; orient to true North; level the weather station            |
| Maintenance            | Recalibration: every 2 years;<br>Cleaning: check for bird droppings and insect debris       |
| Power requirements     | Supply Voltage: 3.6 to 15 V<br>Current draw: 8.0 mA during measurement, 0.3 mA while asleep |
| Operating temperature  | -40 to +50 °C   |
| Communication protocol | SDI-12  |
| Additional equipment   | Pole, stand or tripod and a data logger (third party loggers are compatible too)            |

### 2.2.2 Reference weather station

The performance of the ATMOS41 weather station was evaluated through a comparison with measurements from a meteorological station that serves as a backup station for the official Selhausen (C1) measurement site [Schmidt *et al.*, 2012], which is part of the Integrated Carbon Observation System (ICOS) [ICOS]. The backup station, hereafter referred to as ICOS-bkp, consists of individual, high-quality sensors that fully comply with the ICOS standard. This standard specifies minimum requirements for sensor selection as recommended by the World Meteorological Organization (WMO) [WMO, 2008] and includes detailed descriptions for measurement and calibration processes as well as regular maintenance [Laurent, 2017]. ICOS measurement uncertainty requirements are based on the “achievable uncertainty” that can be expected in

operational practice, as specified in the WMO Guide N° 8 [WMO, 2008]. The total equipment costs for an ICOS level one station are estimated at EUR 10,000 [Brus *et al.*, 2013], including the costs of logger and tripod (ca. EUR 1800 for the Selhausen station). The cost of weather sensors used at an ICOS station is hence more than four times the cost of an ATMOS41 device. The ICOS-bkp station records instantaneous values for solar radiation, temperature, and relative humidity at an interval of 20 s and an installation height of 2.5 m. Precipitation is recorded at a height of 1 m above ground, and a 10 min accumulated value recorded at a separate data logger was used for the comparison with the ATMOS41 stations.

Atmospheric pressure, wind speed, and wind direction are only recorded at the main ICOS station but are not recorded at the backup station. For the comparison of wind speed and direction, data recorded by a Vaisala WXT520 weather transmitter (Vaisala Corporation, Helsinki, Finland) were used. This instrument is installed at a height of 2 m above ground next to the ICOS-bkp station and records data for the SE\_BDK\_002 station of the TERrestrial ENvironmental Observatories network (TERENO) [TERENO, 2020] at a 10 min interval. The Vaisala WXT520 meets the high accuracy and precision standards specified by ICOS for wind speed and direction but has a measurement uncertainty of  $\pm 0.5$  hPa for atmospheric pressure instead of the  $\pm 0.3$  hPa required by ICOS standards. Therefore, the atmospheric pressure sensor at the main ICOS was used as a reference to the ATMOS41 stations.

### **2.2.3 Experimental setup**

Data were collected from 23 April to 5 July 2020 (73 days) in Selhausen, Germany (50.87 N 6.45 E) at an altitude of 103 m a.s.l. The area is characterized by a temperate maritime climate with a mean annual air temperature of 10 °C and annual precipitation of 700 mm. The site is located in an agricultural area with the dominant crops being sugar beet, winter wheat, and winter barley [ICOS, 2020].

Three ATMOS41 weather stations (hereafter referred to as Atmos1, Atmos2 and Atmos3) were set up next to the Vaisala and ICOS-bkp stations. Atmos1 is the first generation of the station, purchased in 2017, and was previously deployed for a period of less than 6 months. Atmos2 and Atmos3 are the latest versions of the station, purchased in 2020, and used for the first time in this study. All three ATMOS41 stations were mounted in a row and installed at 2 m above ground (Figure 2.1). The stations were oriented north and



levelled according to the user manual [METER Group, 2017] to ensure accurate measurements of wind direction, precipitation, and solar radiation. Cumulative or instantaneous data were recorded at a 10 min interval for precipitation and all other variables, respectively. The ATMOS41 stations were connected to a CR1000X data logger (Campbell Scientific Ltd., Logan, UT, USA) which was powered via a 12 V battery connected to a battery charger.

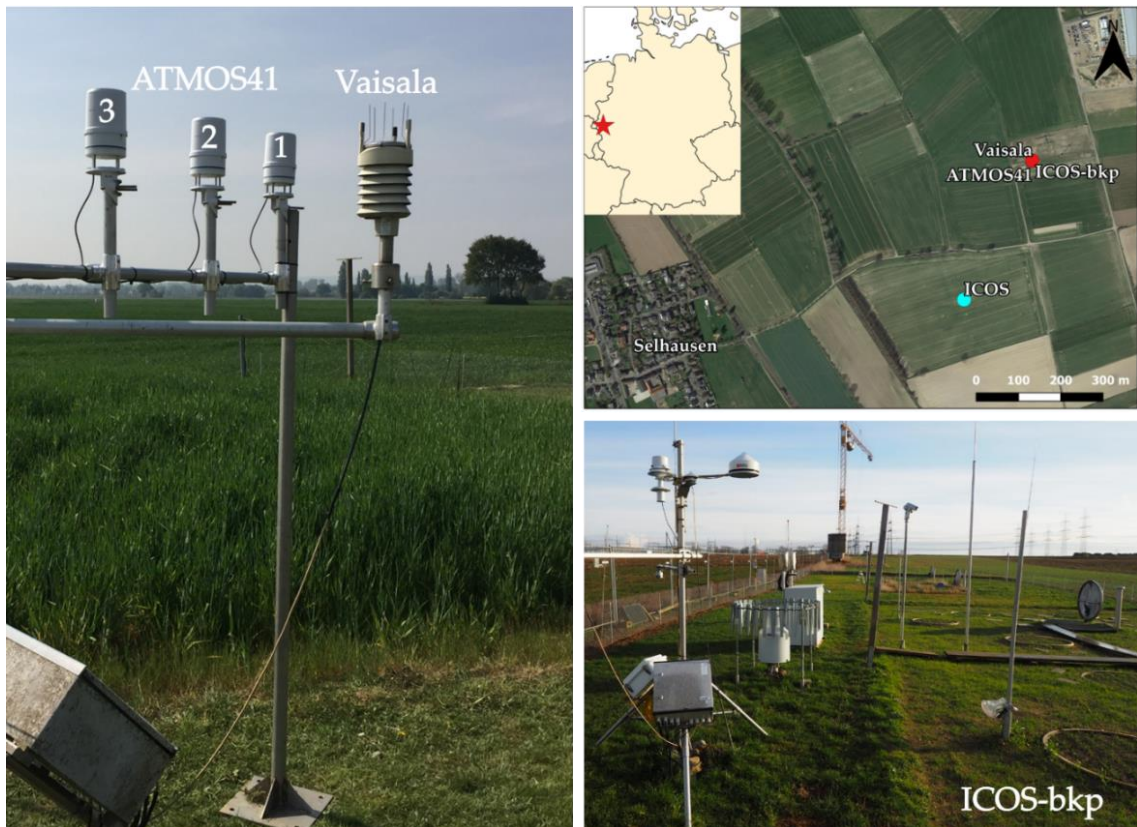


Figure 2.1 Experimental site with the three ATMOS41 stations, the Vaisala weather transmitter and the ICOS-bkp station.

Details on the sensors that measured each variable for the ATMOS41 and for the ICOS-bkp, ICOS or Vaisala stations, including approximate costs for individual sensors used at the reference stations, are listed in Table 2.2. The accuracy of most weather sensors used in the ATMOS41 station, as stated by the manufacturer, is compliant with the “achievable uncertainty” standard used by ICOS, with the exception of the air temperature and atmospheric pressure sensor (ICOS standard of  $\pm 0.1$  °C and  $\pm 0.3$  hPa, respectively).

Table 2.2 Sensor details for the ATMOS41 weather station as well as the ICOS-bkp, Integrated Carbon Observation System (ICOS) or Vaisala station.

| Parameter         | ATMOS41   | ICOS-bkp, ICOS or Vaisala   |
|-------------------|---|---|
| Radiation         | Miniature pyranometer with silicon-cell<br>(Apogee Instruments, Logan, USA)<br>Resolution: 1 W/m <sup>2</sup><br>Accuracy: ±5%                            | Pyranometer with permanent ventilation/heating (CMP21, Kipp & Zonen, Delft, Netherlands; EUR 900)<br>Resolution: 1 W/m <sup>2</sup><br>Accuracy: ±1%                              |
| Precipitation     | Optical sensor rain gauge with 68 cm <sup>2</sup> catch area<br>(METER Group Inc., Pullman, USA)<br>Resolution: 0.017 mm<br>Accuracy: ±5% (up to 50 mm/h) | Weighing rain gauge with 200 cm <sup>2</sup> catch area (Pluvio <sup>2</sup> , Ott HydroMet, Kempten, Germany; EUR 5000)<br>Resolution: 0.05 mm within an hour<br>Accuracy: ±1 mm |
| Temperature       | Thermistor, non-aspirated<br>(METER Group Inc., Pullman, USA)<br>Resolution: 0.1 °C<br>Accuracy: ±0.6 °C  | Resistance thermometer PT100 1/3 Class B (HC2S3, Rotronic, Bassersdorf, Germany; EUR 900)<br>Resolution: 0.01 °C<br>Accuracy: ±0.1 °C   |
| Relative humidity | (METER Group Inc., Pullman, USA)<br>Resolution: 0.1%<br>Accuracy: ±3% (varies with temperature and humidity)  | ROTRONIC <sup>®</sup> Hygromer IN-1 (HC2S3, Rotronic, Bassersdorf, Germany)<br>Resolution: 0.02%<br>Accuracy: ±0.8%   |
| Pressure          | Barometric pressure sensor<br>(METER Group Inc., Pullman, USA)<br>Resolution: 0.1 hPa<br>Accuracy: ±1.0 hPa   | BAROCAP <sup>®</sup> sensor (PTB110, Vaisala Inc., Helsinki, Finland; EUR 730)<br>Resolution: 0.1 hPa<br>Accuracy: ±0.3 hPa (at +20 °C)   |
| Wind speed        | Ultrasonic anemometer<br>(METER Group Inc., Pullman, USA)<br>Resolution: 0.01 m/s<br>Accuracy: the greater of 0.3 m/s or 3%                               | WINDCAP <sup>®</sup> ultrasonic transducer (WXT520, Vaisala Inc., Helsinki, Finland; EUR 2350)<br>Resolution: 0.1 m/s<br>Accuracy: ±3% at 10 m/s                                  |
| Wind direction    | Ultrasonic anemometer<br>(METER Group Inc., Pullman, USA)<br>Resolution: 1°<br>Accuracy: ±5°  | WINDCAP <sup>®</sup> ultrasonic transducer (WXT520, Vaisala Inc., Helsinki, Finland)<br>Resolution: 1°<br>Accuracy: ±3°   |

### 2.2.4 Performance analysis

Python software (version 3.7.6, Python Software Foundation) was used for the graphical and statistical evaluation of the data quality and performance of the ATMOS41 weather station. Data were checked for consistency and erroneous measurements were removed manually. Wind speed and relative humidity were computed according to the procedure described in the ATMOS41 user manual [METER Group, 2017]. Data from the ICOS-bkp and ICOS station were resampled to 10 min instantaneous data for comparison to the ATMOS41 data. Measured atmospheric pressure was corrected for the difference of 3.7

m in observation height (combination of elevation and sensor installation height) between the instrument locations using the barometric formula, while the effect of the distance of 350 m between the stations was considered negligible. Graphical evaluation included time series plots and scatterplots for each parameter. Additionally, residual plots and correlation matrices were obtained and analysed. Residuals were calculated by subtracting the value obtained at the ATMOS41 stations from the value measured at the reference station using hourly mean values (hourly sums for precipitation).

The statistical analysis of solar radiation only considered daytime values as measured nighttime solar radiation was zero. For the evaluation of measured precipitation, all time steps without precipitation were discarded. Statistical analysis of precipitation additionally included an event-based approach using a minimum rainfall amount of  $\geq 0.2$  mm/event and a minimum inter-event time of 1 h.

For statistical comparison, the Arithmetic Mean ( $\mu$ ) of the measured variables was calculated. Other metrics included the Coefficient of Determination ( $R^2$ , Eq. (2.1)) as a measure of agreement between two stations. The Root Mean Square Error (RMSE, Eq. (2.2)) was used as a measure of the difference between two stations. The RMSE is sensible to outliers since higher weights are given to larger deviations between two stations [Walther and Moore, 2005]. The Mean Bias Error (MBE, Eq. (2.3)) was used as a measure of the average error between a station and the reference, with positive values indicating an overestimation and negative values indicating an underestimation. The MBE should be used in combination with other metrics as it is subject to cancellation errors since the sum of positive and negative values may result in a smaller MBE [Ruiz and Bandera, 2017]. Lastly, the Mean Absolute Error (MAE, Eq. (2.4)) was used as a measure of the absolute difference of a measurement compared to the reference measurement. It is not subject to cancellation errors and is less sensitive to outliers compared to the RMSE [Walther and Moore, 2005].

$$R^2 = 1 - \frac{\sum_{i=1}^N (y_i - \hat{y}_i)^2}{\sum_{i=1}^N (\hat{y}_i - \bar{y})^2} \quad (2.1)$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2} \quad (2.2)$$

$$MBE = \frac{\sum_{i=1}^N (y_i - \hat{y}_i)}{N} \quad (2.3)$$

$$MAE = \frac{1}{N} \sum_{i=1}^N |y_i - \hat{y}_i| \quad (2.4)$$

where  $y$  is the reference value,  $\hat{y}$  is the measured value,  $\bar{y}$  is the mean of the reference value, and  $N$  is the number of measurements.

## 2.3 Results and Discussion

### 2.3.1 ATMOS41 inter-sensor variability

Instrument orientation data were recorded in the X- and Y-orientation for all three ATMOS41 stations to identify undesired rotation or tilt. Orientation data (Figure 2.2) showed that all stations remained stable within  $\pm 2$  degrees of dead level in X- and Y-direction as recommended for accurate measurements in the user manual [*METER Group*, 2017]. A few larger tilts that exceed the  $\pm 2$  degrees mark are observed in Figure 2.2, which mostly coincide with wind speeds  $> 6$  m/s (data not shown). However, only  $\sim 0.3\%$  of measurements were affected for Atmos2 and Atmos3 and large tilts were never sustained for more than a few measured time steps. For Atmos1, a larger 2.6% of measurements were affected due to a small, temporary change in orientation between 24 and 29 April 2020, which was likely caused by a movement of the whole mounting structure. In addition, Atmos1 showed a slight misalignment of 0.5 to 1.0 degrees compared to Atmos2 and Atmos3, which was not considered significant.

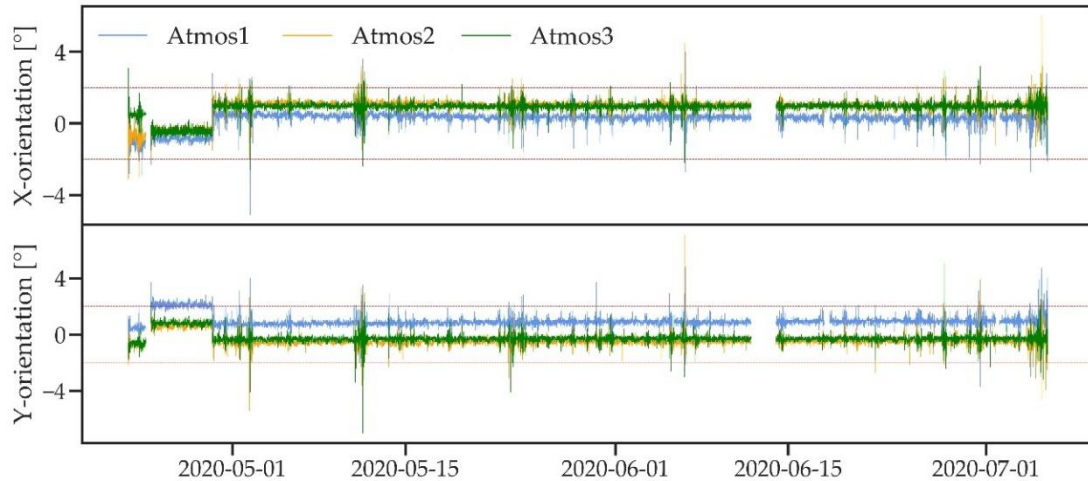


Figure 2.2 X- and Y-orientation for the three ATMOS41 weather stations. The red dotted line indicates  $\pm 2$  degrees from dead level.

The inter-sensor variability of the three ATMOS41 stations was analysed for the entire observation period (23 April to 5 July 2020) for all standard weather variables by examining 10 min instantaneous data. Figure 2.3 shows a pairwise comparison of the three stations using scatterplots, histograms with probability density functions, and the  $R^2$  value arranged in a matrix. The scatterplots show good agreement and no apparent bias between stations, with most of the data points lying in the proximity of the identity line. Some scattering effect can be observed for solar radiation (Figure 2.3a), which may have been caused by temporal shading of a single sensor or differences in response time to changing radiation. Relatively strong scatter can be observed in the wind speed measurements (Figure 2.3f), which was likely caused by other external effects such as small-scale turbulences around the stations. This scatter is reduced considerably when the data are aggregated to a larger time step (data not shown). The histograms and probability density functions of all measured variables generally show very similar distributions. Only in the case of relative humidity (Figure 2.3e) does Atmos1 show small differences in the distribution of values compared to the histograms of Atmos2 and Atmos3.

The comparison of all variables shows an  $R^2 \geq 0.96$  except for wind speed, for which the  $R^2$  ranges between 0.72 and 0.74.  $R^2$  values increase when hourly averages are considered (data not shown), especially in the case of wind speed ( $R^2$  increases to 0.91 for Atmos1 vs. Atmos2, 0.92 for Atmos1 vs. Atmos3, and 0.90 for Atmos2 vs. Atmos3). Despite most comparisons being rather satisfactory, there is slightly better agreement between Atmos2 and Atmos3 when compared to Atmos1 for solar radiation, atmospheric pressure, and relative humidity.

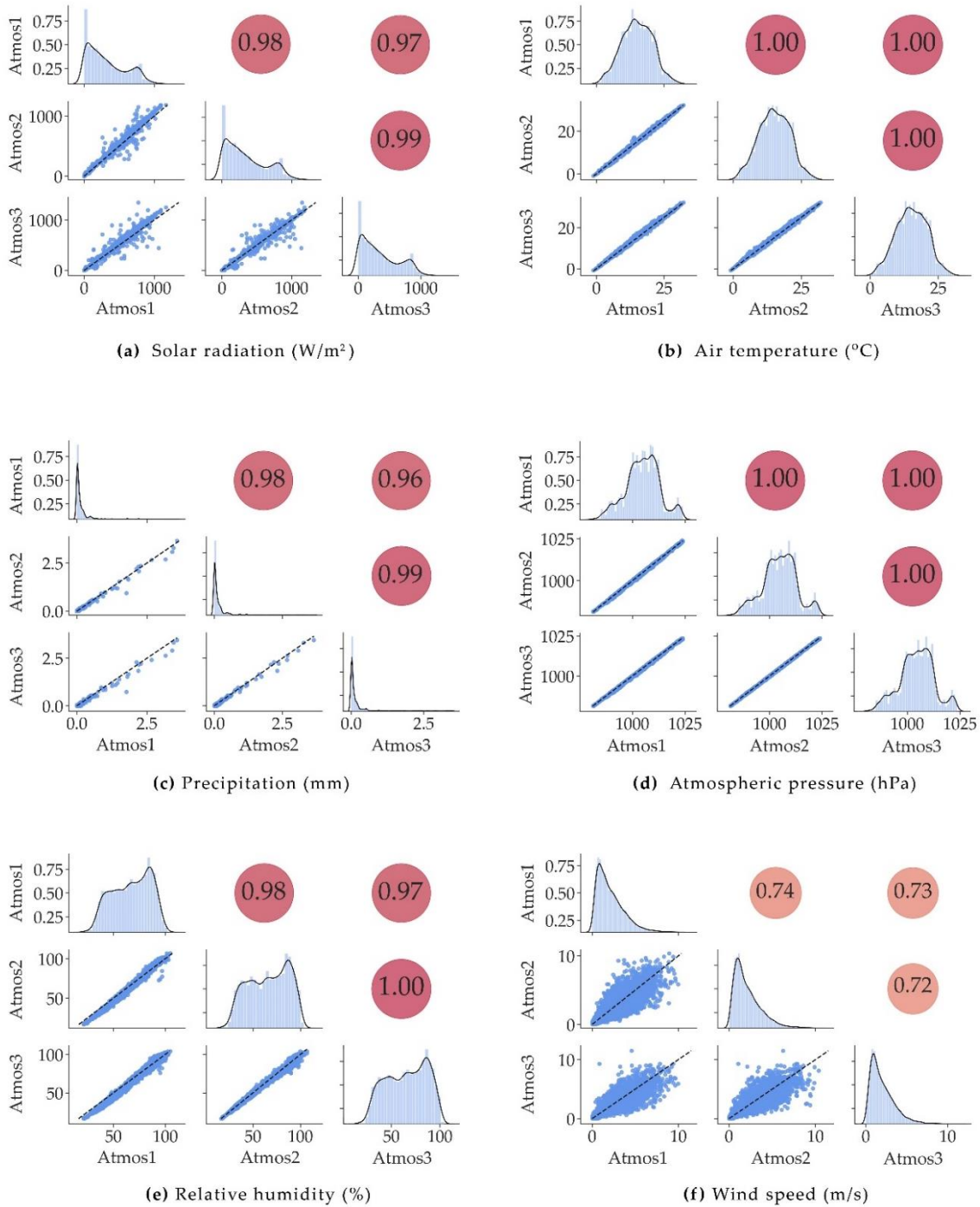


Figure 2.3 (a–f) Correlation matrices for all weather variables measured by the three ATMOS41 stations. Subplots in the lower left show scatterplots of station pairs with the dashed line indicating the 1:1 identity line, the diagonal shows histograms of measured values with probability density functions, upper right shows the coefficient of determination  $R^2$ .

A statistical summary with a pairwise assessment of all three ATMOS41 stations is given in Table 2.3. There is generally close agreement between all stations for most parameters with low RMSE and small MBE. Larger variability within the three stations was observed for wind speed and precipitation measurements. RMSE for wind speed is  $\sim 0.76$  m/s at an average wind speed between 2.02 and 2.11 m/s. Atmos1 and Atmos2 measured on

average slightly higher wind speed compared to Atmos3 as shown by the mean and MBE. Precipitation measurements show a RMSE of  $\sim 0.06$  mm at an average precipitation between 0.17 and 0.20 mm. The variability in precipitation measurements becomes more apparent when comparing the total precipitation amounts, which were unusually low for the observed months from late April to early July. The total amounts are 82.21 mm (Atmos1), 75.92 mm (Atmos2), and 70.79 mm (Atmos3), while long-term monthly means (1981–2010) are between 47 and 77 mm for the same months [DWD, 2021]. The difference between the three stations is considerable given the relatively short observation period and low total rainfall and stands in contrast to the test measurements performed by METER, where a difference of  $< 20$  mm was observed within three ATMOS41 stations for a total of  $\sim 800$  mm of rainfall over a period of 4 months [METER Group, 2018]. The results suggest that wind-induced random errors such as the deflection of air flow and the formation of eddies and turbulences around the gauges [Sieck *et al.*, 2007] had an important effect on the measurements. Atmos1 was positioned west-southwest of the other two stations, which was identified as the prominent wind direction during rainfall (data not shown). The three stations may have perturbed each other due to their alignment with respect to the wind direction and the relatively small distance between the stations, thus increasing the above-mentioned wind effects for Atmos2 and even more for Atmos3. This could explain the consistently lower amounts of rainfall measured by Atmos2 and Atmos3 compared to Atmos1. Low rainfall rates, as observed for most of the measurement period, show a high volumetric fraction of smaller drops (diameter  $< 1$  mm), which are particularly prone to wind induced errors [Nešpor and Sevruk, 1999]. This may have caused the large observed variability despite the relatively low wind speeds observed during rainfall events and throughout the measurement period ( $\sim 2$  m/s).

Generally, somewhat lower RMSE and MBE were observed between Atmos2 and Atmos3 as opposed to Atmos1 for solar radiation, atmospheric pressure, and relative humidity. The greater similarity between the newer ATMOS41 variants with regard to the latter two variables is most likely a result of the sensor improvements implemented after 2017, as mentioned above. However, the most pronounced difference was observed for solar radiation, where a bias of  $\sim -25$  W/m<sup>2</sup> was found between the older Atmos1 (2017 version) and the newer ATMOS41 stations. In comparison, the bias between Atmos2 and Atmos3 was only  $-0.39$  W/m<sup>2</sup> (Table 2.3).

Table 2.3 Statistical summary of the inter-sensor comparison for all standard weather variables measured by three ATMOS41 weather stations. Colours give an evaluation of the comparison, with red indicating the lowest and green the highest performance.

| Station °N<br>Parameter             | $\mu$             |                   |                   | RMSE    |         |         | MBE     |         |         |
|-------------------------------------|-------------------|-------------------|-------------------|---------|---------|---------|---------|---------|---------|
|                                     | 1                 | 2                 | 3                 | 1 vs. 2 | 1 vs. 3 | 2 vs. 3 | 1 vs. 2 | 1 vs. 3 | 2 vs. 3 |
| Solar radiation [W/m <sup>2</sup> ] | 320.26            | 345.21            | 345.6             | 38.34   | 47.37   | 32.76   | -24.96  | -25.35  | -0.39   |
| Precipitation [mm]                  | 0.20<br>(82.21) * | 0.18<br>(75.92) * | 0.17<br>(70.79) * | 0.06    | 0.08    | 0.05    | 0.015   | 0.027   | 0.012   |
| Air temperature [°C]                | 15.05             | 15.11             | 15.26             | 0.22    | 0.38    | 0.34    | -0.07   | -0.22   | -0.15   |
| Atmospheric pressure [hPa]          | 1004.92           | 1004.70           | 1004.53           | 0.42    | 0.51    | 0.23    | 0.22    | 0.39    | 0.17    |
| Relative Humidity [%]               | 67.35             | 66.18             | 65.56             | 3.26    | 3.49    | 1.38    | 1.17    | 1.79    | 0.62    |
| Wind speed [m/s]                    | 2.1               | 2.11              | 2.02              | 0.77    | 0.75    | 0.76    | -0.009  | 0.089   | 0.098   |

\* values in parentheses refer to the total precipitation amount during the observation period.

At first, the ageing of the pyranometer was considered as a possible explanation for the better agreement between the two newer ATMOS41 stations. This assumption was tested using previous data from the older Atmos1 (2017 version). Between 12 December 2017 and 24 May 2018 (164 days), the station was set up next to the ICOS site in Selhausen, 350 m from the ICOS-bkp station (Figure 2.1). Graphical and statistical analysis showed minor differences in the performance of the station between the two periods (data not shown), which is more likely a result of the different seasons and lengths of the two observation periods. The results suggest a stable performance of the Atmos1 over the 3-year period, even though calibration or maintenance were not performed. However, Atmos1 did not operate continuously throughout this period and hence it was not exposed to adverse weather conditions, such as strong solar radiation or heavy wind and precipitation. Therefore, sensor ageing or deterioration should be further studied, especially when continuous deployment of the station as part of a large monitoring network such as TAHMO is intended. A long-term assessment could include field visits, calibration checks and the establishment of statistical validation procedures as proposed in [Estévez *et al.*, 2011] or, if possible, comparison with a nearby reference station over an extended period.

Communication with the manufacturer allowed us to identify another possible issue related to the pyranometer provided by Apogee Instruments. A problem in the production of the early pyranometers was identified, which affected some of the earlier weather



stations and was solved at a later stage. This most likely explains the observed difference in performance between the older Atmos1 (2017 version) and the more recent Atmos2 and Atmos3 stations.

### **2.3.2 Comparison of ATMOS41 with ICOS backup station**

In the following, data collected over the 73-day period that includes late spring and early summer months with a small data gap of two days in mid-June are compared. The first three weeks of radiation data for Atmos3 were missing due to a defect funnel that was later replaced. To better visualize the comparison of the different stations, only a period of eight days from 30 May to 6 June (23 April to 5 July for precipitation) is shown in this section. The full time series can be found in the Appendix (Figure A.1).

Table 2.4 shows a summary of the statistical performance analysis of the three ATMOS41 stations compared to the reference station. Overall,  $R^2 > 0.90$  and relatively low RMSE, MBE and MAE were found for most variables except precipitation, wind speed, atmospheric pressure and solar radiation (only Atmos1). In the following, each variable is assessed in more detail.

Table 2.4 Statistical summary of the performance of three ATMOS41 stations compared to the ICOS-bkp or Vaisala reference station. Colours give an evaluation of the comparison, with red indicating the lowest and green the highest performance.

| Variable                            | R <sup>2</sup> |      |      | RMSE  |       |       | MBE    |       |        | MAE   |       |       |
|-------------------------------------|----------------|------|------|-------|-------|-------|--------|-------|--------|-------|-------|-------|
|                                     | 1              | 2    | 3    | 1     | 2     | 3     | 1      | 2     | 3      | 1     | 2     | 3     |
| Solar radiation (W/m <sup>2</sup> ) | 0.96           | 0.99 | 0.99 | 56.46 | 31.88 | 32.28 | -35.22 | -9.03 | -10.06 | 38.14 | 18.40 | 17.14 |
| Precipitation (mm/10min)            | 0.92           | 0.93 | 0.93 | 0.13  | 0.13  | 0.13  | 0.02   | -0.01 | -0.02  | 0.08  | 0.09  | 0.08  |
| Precipitation (mm/event)            | 0.99           | 0.99 | 0.99 | 0.19  | 0.24  | 0.30  | 0.06   | -0.05 | -0.17  | 0.11  | 0.15  | 0.21  |
| Temperature (°C)                    | 0.99           | 0.99 | 0.99 | 0.53  | 0.49  | 0.45  | -0.37  | -0.31 | -0.16  | 0.42  | 0.38  | 0.33  |
| Atmospheric Pressure (hPa)          | 0.98           | 0.99 | 1.00 | 1.17  | 0.89  | 0.75  | 1.01   | 0.79  | 0.63   | 1.02  | 0.80  | 0.64  |
| Relative Humidity (%)               | 0.95           | 0.97 | 0.97 | 4.33  | 3.36  | 3.39  | 1.37   | 0.25  | -0.36  | 3.47  | 2.50  | 2.55  |
| Wind speed (m/s)                    | 0.62           | 0.58 | 0.63 | 0.84  | 0.88  | 0.82  | 0.17   | 0.18  | 0.09   | 0.55  | 0.59  | 0.55  |

### 2.3.2.1 Solar radiation

Figure 2.4a shows an 8-day period of solar radiation as measured by the four weather stations. The timing and variability of radiation during the day are well captured by the ATMOS41 stations. However, the maximum measured solar radiation is slightly lower than that of the reference station, especially for Atmos1. On a clear day, Atmos3 shows a recurring small drop in solar radiation in the early morning, suggesting a shadow cast from a surrounding sensor. On overcast days such as 4 June, the four stations show almost identical measurements.

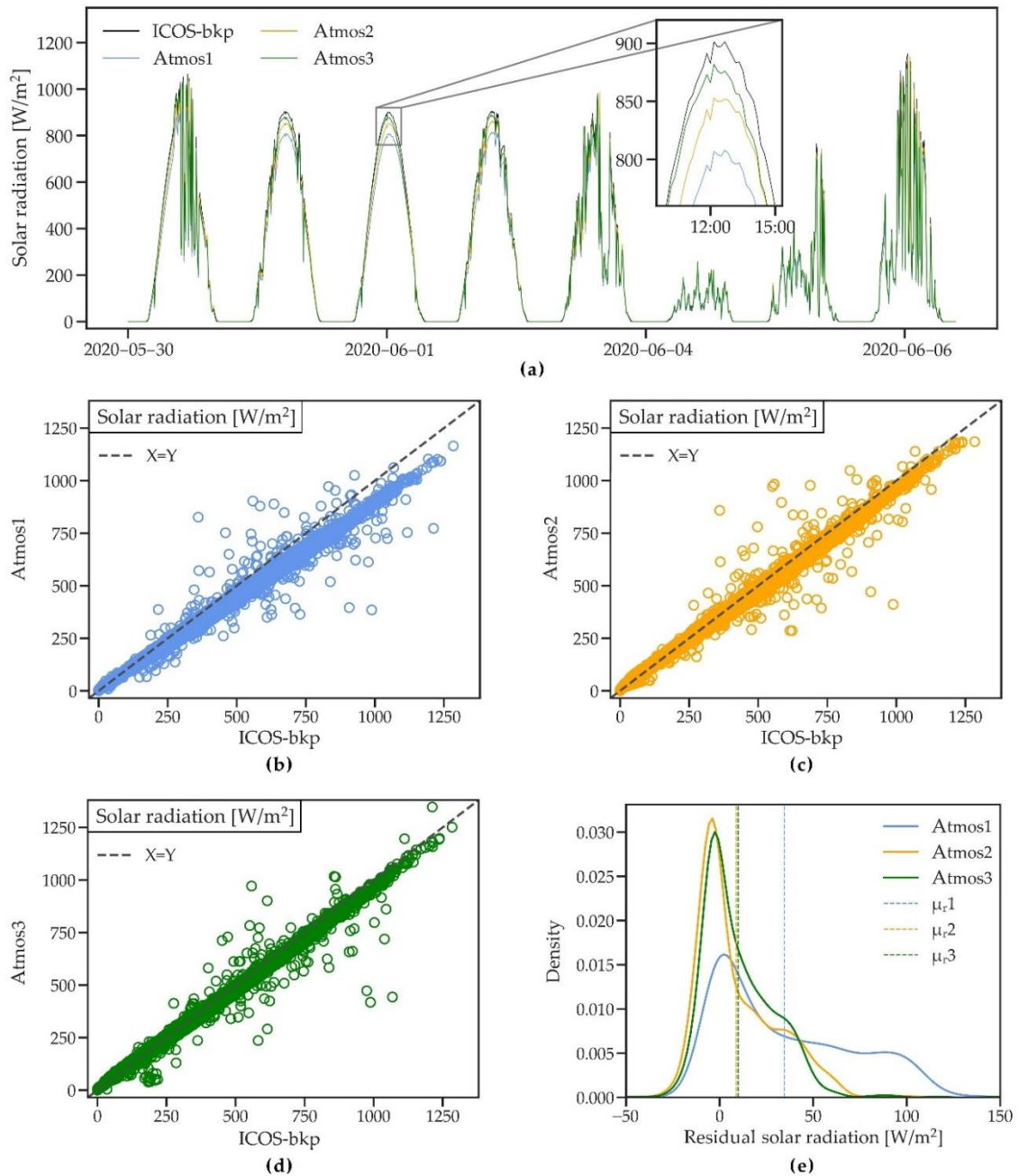


Figure 2.4 (a) A short time series of solar radiation measured by three ATMOS41 weather stations and the ICOS-bkp station from 30 May to 6 June 2020. (b–d) Scatterplots of 10 min solar radiation for the three ATMOS41 stations vs. the reference station. (e) Probability density functions of the residual mean hourly solar radiation. Dashed lines show the mean of residuals ( $\mu_r$ ).

The scatterplots of the ATMOS41 station vs. the ICOS-bkp (Figure 2.4b–d) confirm the overall good agreement of the stations, with an  $R^2$  between 0.96 and 0.99 (Table 2.4). The plots show little scatter and RMSE is  $\sim 32$  W/m<sup>2</sup> for Atmos2 and Atmos3 and somewhat higher for Atmos1 (56.46 W/m<sup>2</sup>) (Table 2.4). Solar radiation values  $> 400$  W/m<sup>2</sup> show a small underestimation by the ATMOS41 (Figure 2.4b–d).

Figure 2.4e depicts the deviation between the three ATMOS41 stations and the ICOS-bkp station through a probability density plot of the residuals from hourly average data, which considers only daytime solar radiation. The peaks of the distributions show a small tendency of the ATMOS41 stations to measure higher values (negative residuals), which occurs at lower solar radiation as suggested by the scatterplots (Figure 2.4b–d). The underestimation of high solar radiation is represented in the right tail of the distribution (positive residuals), with a mean bias of  $-35.22 \text{ W/m}^2$  for Atmos1 and mean biases of  $-9.03$  and  $-10.06 \text{ W/m}^2$  for Atmos2 and Atmos3, respectively (Table 2.4).

The presented results for the Atmos1 generally agree well with the analysis by [Anand and Molnar, 2018], which compared the 2017 version of the ATMOS41 station with a SwissMetNet station. In their study, a lower bias of 8.9% was found compared to the one in this comparison (9.9%). This may be attributed to the overall lower radiation during the winter period studied by [Anand and Molnar, 2018] as opposed to the early summer period of this study that included many sunny days. Despite the 2 km distance between pyranometers, the authors observed a lower MAE and RMSE ( $13.57$  and  $39.40 \text{ W/m}^2$ ) than what was found in this study, which may again be related to the characteristics of the observation period since the ATMOS41 measures more accurately in the lower radiation range.

Despite the small systematic deviation from the reference ICOS-bkp station, the quality of the radiation measurements provided by the ATMOS41 was satisfactory. The newer stations show considerable improvement compared to the 2017 version of the station (Atmos1) and confirm the comparison test performed by the manufacturer, where a linear regression ( $y = 1.0323x$ ) showed  $\sim 3\%$  underestimation [METER Group, 2018]. Linear regressions for Atmos2 ( $y = 1.0372x$ ) and Atmos3 ( $y = 1.0336$ ) were similar to the one found by METER (Figure A.2). Granting that this bias persists in other climates and locations and compared to other high-performance pyranometers, a simple linear correction function may be developed and used to adjust the measurements.

### **2.3.2.2 Precipitation**

Figure 2.5a shows an 8-day period with several precipitation events between 28 April and 4 May. The timing of the events agrees well for all four stations, but there are some differences in magnitude and the effect of the different measurement resolutions ( $0.017 \text{ mm}$  for the ATMOS41 and  $0.05 \text{ mm}$  within an hour for the Pluvio<sup>2</sup> that is used at the

ICOS-bkp station) is visible. A direct comparison of the rainfall measured by the two gauges is complicated given the difference in measurement resolution, gauge size and shape, and installation height, as well as the use of a windshield with the Pluvio<sup>2</sup>. The difference in resolution caused a greater scatter for small rainfall amounts in the 10 min time series (Figure 2.5b), with an  $R^2 \sim 0.9$ , RMSE  $\sim 0.15$ , and MAE  $\sim 0.10$  mm for the three stations. The event-based analysis compared 46 rainfall events with rainfall amounts ranging between 0.2 and 19.5 mm and showed more coherent results with  $R^2 \sim 0.99$  (Figure 2.5c). On average, Atmos1 measured higher precipitation, Atmos3 measured somewhat lower precipitation, while Atmos2 showed the least bias compared to the reference station (Table 2.4).

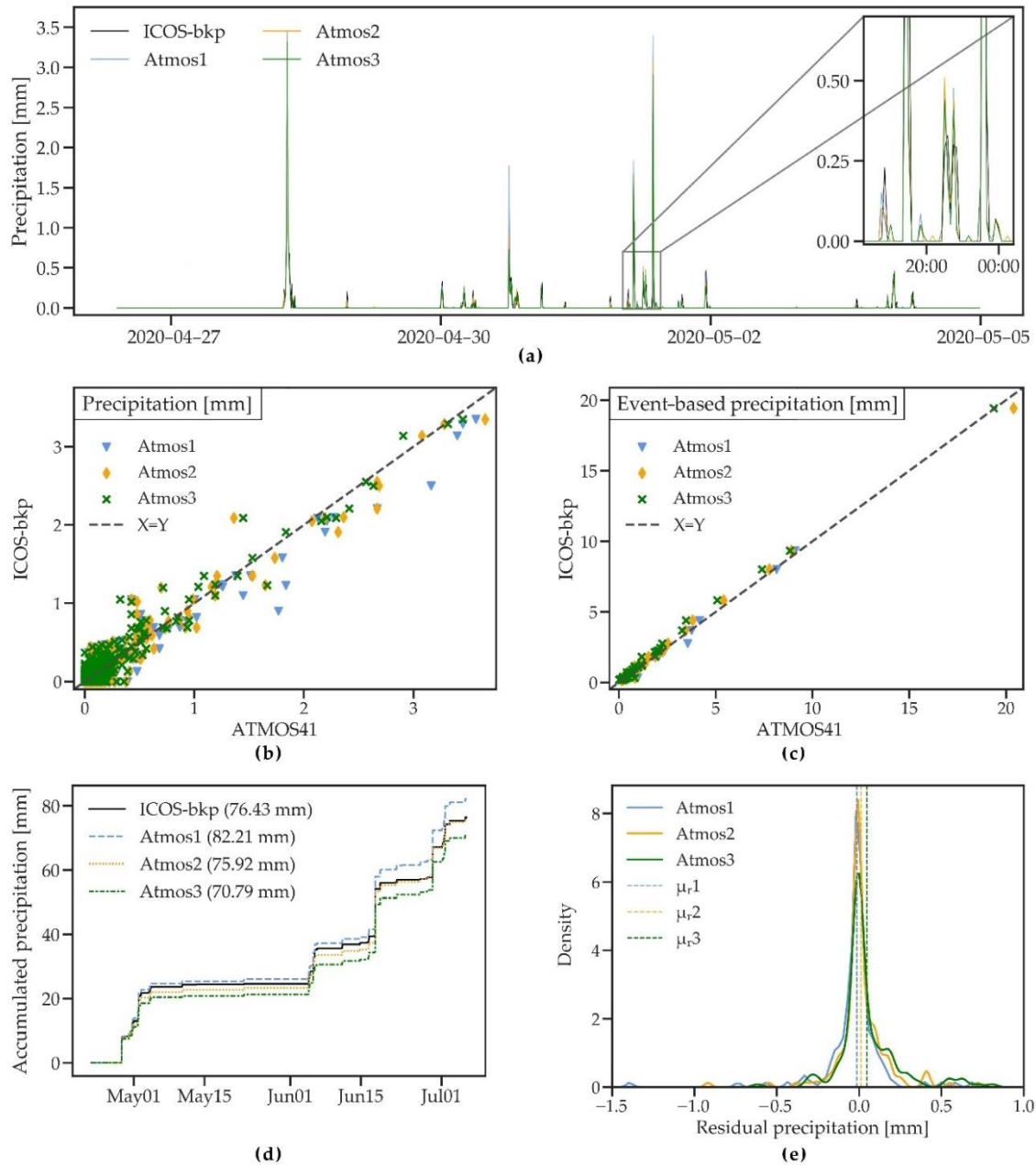


Figure 2.5 (a) A short time series of precipitation measured by three ATMOS41 weather stations and the ICOS-bkp station from 28 April to 4 May 2020. (b,c) Scatterplots of 10 min precipitation and event-based precipitation sum for the three ATMOS41 stations vs. the reference station. (d) Cumulative precipitation measured by the three ATMOS41 weather stations and the reference station for the whole time series (numbers in parentheses refer to total precipitation amount). (e) Probability density functions of the residual hourly precipitation sum. Dashed lines show the mean of residuals ( $\mu_r$ ).

Differences between the stations are more apparent when the cumulative precipitation for the observation period is analysed (Figure 2.5d). Total differences in precipitation compared to the reference are 5.78 mm (7.56%), -0.51 mm (-0.67%), and -5.64 mm (-7.38%) for Atmos1, Atmos2, and Atmos3. The difference to the reference rain gauge and between the ATMOS41 stations (as discussed in Section 2.3.1) is considerable and shows higher discrepancies than what is reported by the manufacturer (within 3% of the

average of three tipping-spoon rain gauges) [METER Group, 2018]. Surprisingly, *Anand and Molnar* [2018] found an underestimation of only 8.7%, even though their observation period included the entire winter season with several snowfall events. Since the ATMOS41 rain gauge is not heated and solid precipitation first needs to melt before it can be measured, higher errors could be expected during that period. This could not be further investigated, since snow was not observed during the measurement period of the present study. However, many applications such as agricultural monitoring or the use of the station in snow free climates do not rely on accurate measurements of the volume of solid precipitation.

As previously discussed in Section 2.3.1, wind-induced errors have likely played an important role in the measurement of rainfall, leading to significant errors considering the relatively small total precipitation amount and low rainfall intensities that were characteristic for the observed period. Additionally, gauge size and shape influence the deformation of the wind field at the gauge and minor changes in installation height can cause differences of up to 10% in precipitation measurements, as comparison studies of different rainfall gauges have shown [*Nešpor and Sevruck, 1999; Sevruck and Klemm, 1989*]. A higher wind-induced under catch could therefore be expected for the ATMOS41 stations that were installed at an approximate height of 2 m compared to the Pluvio<sup>2</sup> that is installed at a height of 1 m and uses an Alter windshield which has shown to improve the performance of the gauge [*Colli et al., 2016; Kochendorfer et al., 2017*]. The higher precipitation amount measured by the Atmos1 could be a result of the frequent detection of very small rainfall amounts, since the Pluvio<sup>2</sup> does not measure fine precipitation below a threshold of 0.05 mm within an hour.

Rainfall intensity during the observation period rarely exceeded 10 mm/h, a commonly used threshold for heavy rainfall [*DWD, 2020*]. Those events did not show lower accuracy of the ATMOS41 station, but a longer observation period with higher rainfall intensities is needed to accurately assess the performance of the station during extreme events.

### **2.3.2.3 Air temperature**

Figure 2.6a shows air temperature data of the four stations during an 8-day period. Temperature dynamics are well captured by all ATMOS41 stations. However, daily maximum temperature and temperature during rainfall (5 June) are slightly lower and show a higher noise level for the ATMOS41 stations. The latter could be a result of a wet,

exposed temperature sensor or its immediate surroundings, making it more prone to evaporative cooling compared to the shielded ICOS-bkp sensor. In comparison, *Anand and Molnar* [2018] found that night-time lows measured by the ATMOS41 were generally lower compared to the IAC instrument, while showing high relative humidity. The authors observed temperatures ranging from  $-13$  to  $23$  °C with a mean temperature of  $4.5$  °C, as opposed to the mean temperature of  $15$  °C measured during the present study. The scatterplots (Figure 2.6b–d) and statistical analysis (Table 2.4) show very good performance of the ATMOS41 with values close to the identity line, little scatter, and  $R^2$  close to 1. RMSE and MAE are between  $0.33$  and  $0.53$  °C for all stations, nearly 50% lower than the RMSE and MAE reported in *Anand and Molnar* [2018].

Similar to the findings of *Anand and Molnar* [2018], there is a small mean bias towards lower temperature measured by the ATMOS41 (MBE between  $-0.16$  and  $-0.37$  °C), as also reflected in the probability density plot of the hourly residuals (Figure 2.6e). The temperature sensor of the ATMOS41 is exposed to solar heating, which is why an energy balance correction is used to calculate the actual temperature. The correction factor is proportional to solar radiation and inversely proportional to wind speed. Since errors in the measurement of those two variables may propagate to the temperature measurement, the overestimation of wind speed may explain the small bias in the measurement (Table 2.4). However, most values lie within  $0.5$  °C difference. Additionally, no tendency to lower accuracy with temperatures  $> 30$  °C was identified, which suggests that the ATMOS41 measurements are reliable within the observed range of  $-1.1$  to  $32.2$  °C. Even though the accuracy of  $\pm 0.6$  °C, as stated by the manufacturer, does not meet the “achievable uncertainty” standard of  $\pm 0.2$  °C used by ICOS, air temperature measurements with the ATMOS41 were reliable and consistent.



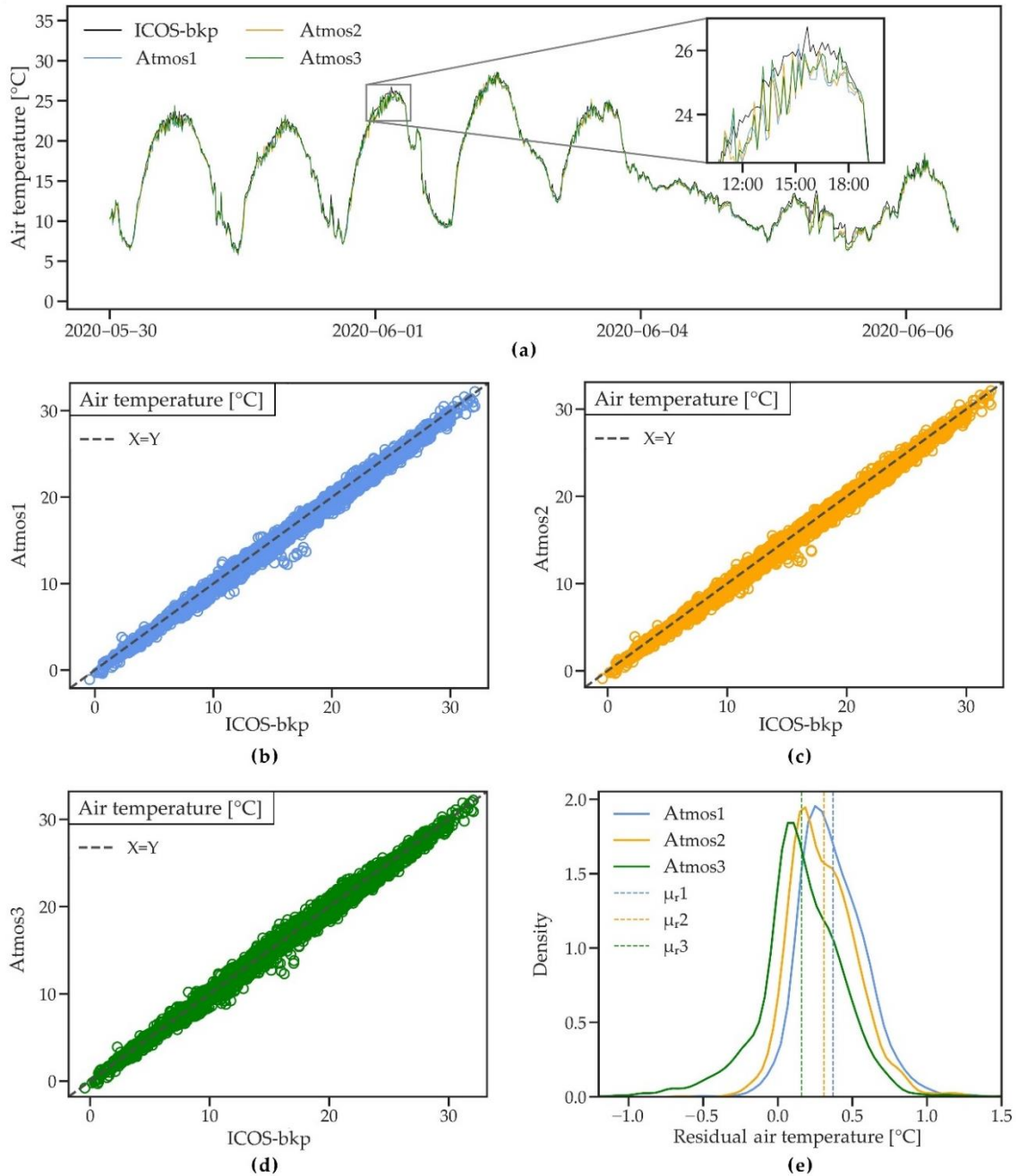


Figure 2.6 (a) A short time series of air temperature measured by three ATMOS41 weather stations and the ICOS-bkp station from 30 May to 6 June 2020. (b–d) Scatterplots of 10 min air temperature for the three ATMOS41 stations vs. the reference station. (e) Probability density functions of the residual mean hourly air temperature. Dashed lines show the mean of residuals ( $\mu_r$ ).

### 2.3.2.4 Atmospheric pressure

Figure 2.7a shows atmospheric pressure measured by the four stations during an 8-day period. The ATMOS41 stations closely follow the reference station with small differences that are consistently found during daily peaks and at lower pressures, which generally coincide with rainfall. The high  $R^2 \geq 0.97$  indicates good agreement of the measurements. However, RMSE and MAE are relatively large, ranging between 0.75 and 1.17 hPa and

0.64 and 1.02 hPa, respectively. In agreement with *Anand and Molnar* [2018], the scatterplots (Figure 2.7b–d) and the probability density plot (Figure 2.7e) show a small bias towards higher values measured by the ATMOS41 compared to the reference station (MBE between 0.63 and 1.01 hPa). Atmos1 shows slightly lower overall performance, which was likely improved as a consequence of the secondary calibration added for the newer stations (see Section 2.1). While the ATMOS41 performs satisfactorily within the manufacturer stated accuracy of  $\pm 1$  hPa, the pressure sensor does not meet the “achievable uncertainty” requirement of 0.3 hPa as commissioned by the WMO [WMO, 2008]. Therefore, the ATMOS41 shows only moderate performance in measuring atmospheric pressure compared to the reference station.

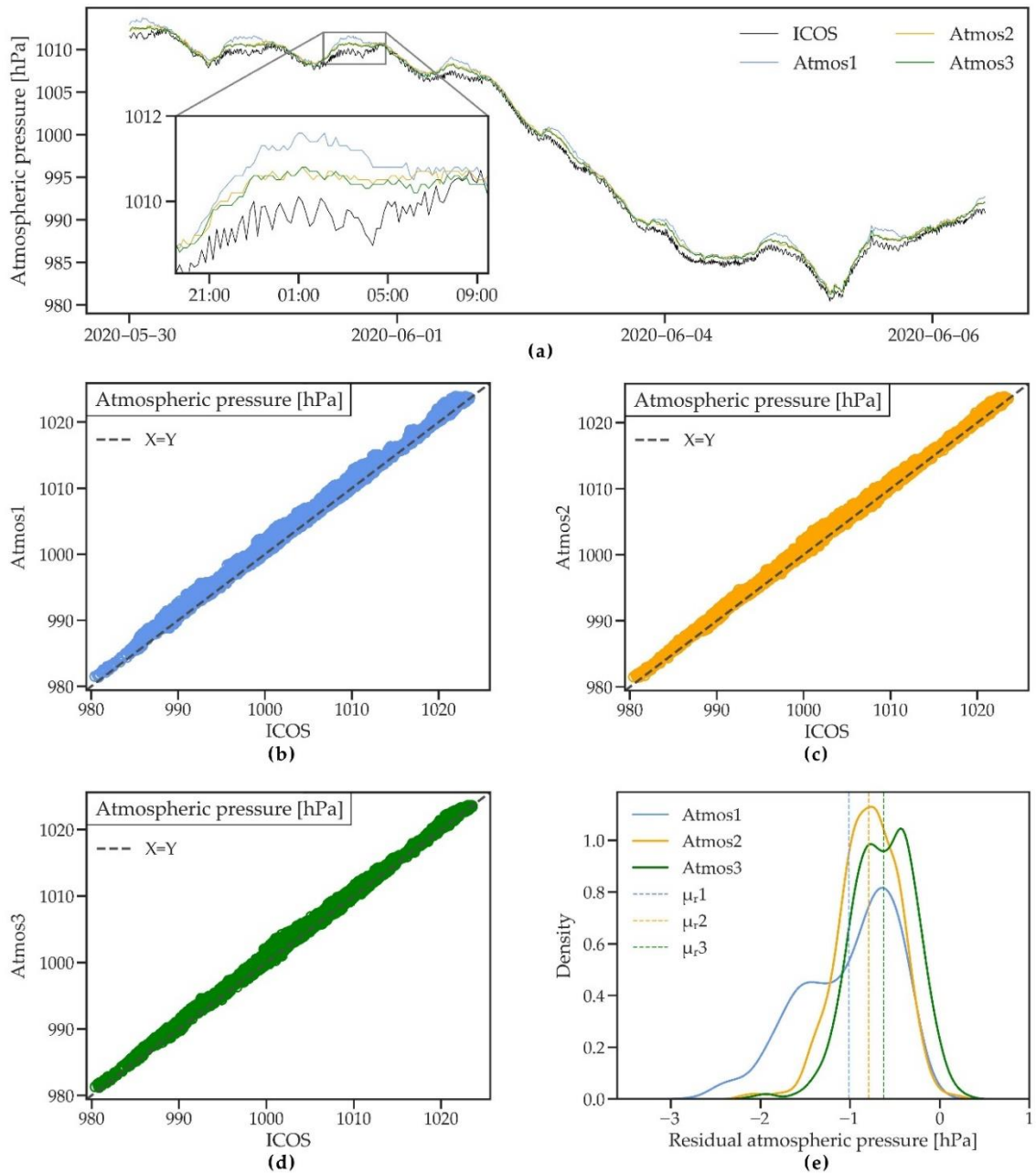


Figure 2.7 (a) A short time series of atmospheric pressure measured by three ATMOS41 weather stations and the ICOS-bkp station from 30 May to 6 June 2020. (b–d) Scatterplots of 10 min atmospheric pressure for the three ATMOS41 stations vs. the reference station. (e) Probability density functions of the residual mean hourly atmospheric pressure. Dashed lines show the mean of residuals ( $\mu_r$ ).

### 2.3.2.5 Relative humidity

Figure 2.8a shows relative humidity as measured by all four stations during an 8-day period of the measured time series. Relative humidity is captured well by the ATMOS41, with slightly higher humidity measured only during rain events such as 5 June for all ATMOS41 stations. This matches the observed small underestimation of temperature during rain events, as discussed in Section 2.3.2.3. Atmos1 additionally shows higher values during the daytime minimum humidity. The statistical summary (Table 2.4) shows  $R^2 \geq 0.95$  for all stations and RMSE and MAE range from 3.4 to 4.3% and 2.5 to 3.5%, respectively, with Atmos1 showing slightly poorer performance than Atmos2 and Atmos3.

The scatterplot for Atmos1 (Figure 2.8b) confirms a small bias towards higher values for lower relative humidity and towards lower values when humidity is high. As a result, the Atmos1 shows a relatively higher MBE of 1.37% compared to Atmos2 and Atmos3 (MBE of 0.25 and  $-0.36\%$ , respectively). This indicates that the manufacturer's adaptation of the calibration function (see Section 2.3.1) for the newer stations resulted in an improvement compared to the older Atmos1 (2017 version). The probability density plot of the residuals (Figure 2.8e) confirms the improved performance of the newer stations.

The ATMOS41 stations tend to saturate at 100% relative humidity more frequently than the reference station, which seems to verify the observation of *Anand and Molnar* [2018] and which may also be related to the underestimation of air temperature, as discussed in Section 2.3.2.3.

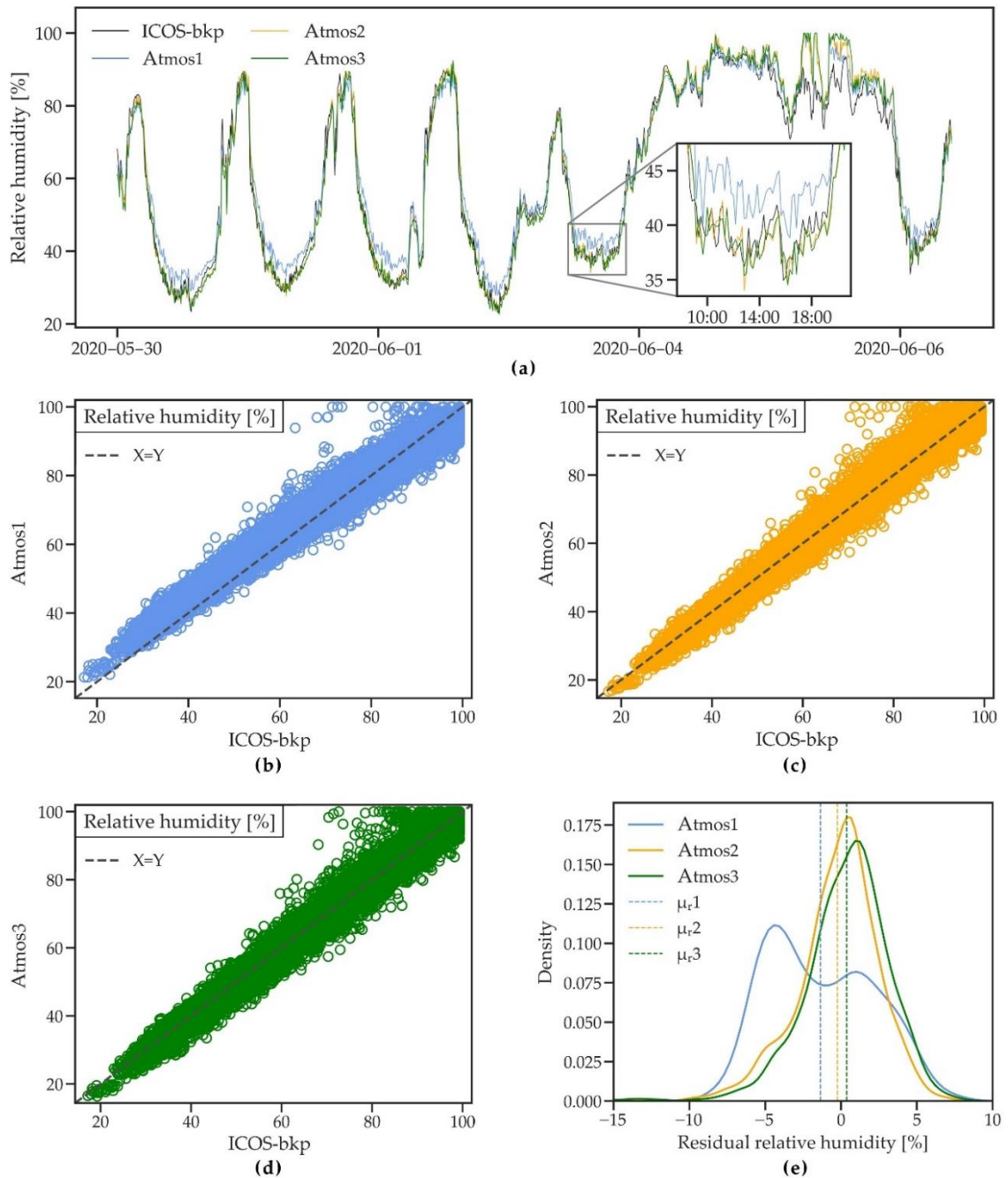


Figure 2.8 (a) A short time series of relative humidity measured by three ATMO541 weather stations and the ICOS-bkp station from 30 May to 6 June 2020. (b–d) Scatterplots of 10 min relative humidity for the three ATMO541 stations vs. the reference station. (e) Probability density functions of the residual mean hourly relative humidity. Dashed lines show the mean of residuals ( $\mu_r$ ).

### 2.3.2.6 Wind speed and direction

Figure 2.9a shows wind speed measured by the four stations during an 8-day period. Daily wind dynamics measured by the three ATMO541 stations match well with the measurements of the Vaisala station. However, measurements by the ATMO541 show higher peak values and a larger variability compared to the Vaisala station, which can be explained by the finer resolution of the anemometer of the ATMO541.

The scatterplots (Figure 2.9b–d) show relatively large scatter around the identity line, with an  $R^2$  between 0.58 and 0.63. The wide spread in wind measurements is likely a result of small-scale turbulence caused by surrounding instruments, as discussed in the context of the precipitation measurements in Section 2.3.2.2 and which are captured due to the rapid response of ultrasonic anemometers to sudden changes in wind speed [Ammann, 1994].  $R^2$  increases up to 0.89 when hourly averages are considered, suggesting that the scatter can be reduced when small-scale differences average out over larger periods. RMSE and MAE are  $\sim 0.9$  and  $\sim 0.6$  m/s, respectively (Table 2.4). The probability density plot of the residuals (Figure 2.9e) shows a small mean overestimation of wind speed (negative residuals) with MBE between 0.09 and 0.18 m/s, with Atmos3 showing the best performance. Both station types used in this comparison use ultrasonic anemometers, which can measure very low wind speeds. Therefore, the agreement found in this comparison was higher than that of *Anand and Molnar* [2018], where the ATMOS41 was compared to a cup anemometer that records zero wind speed values more frequently.

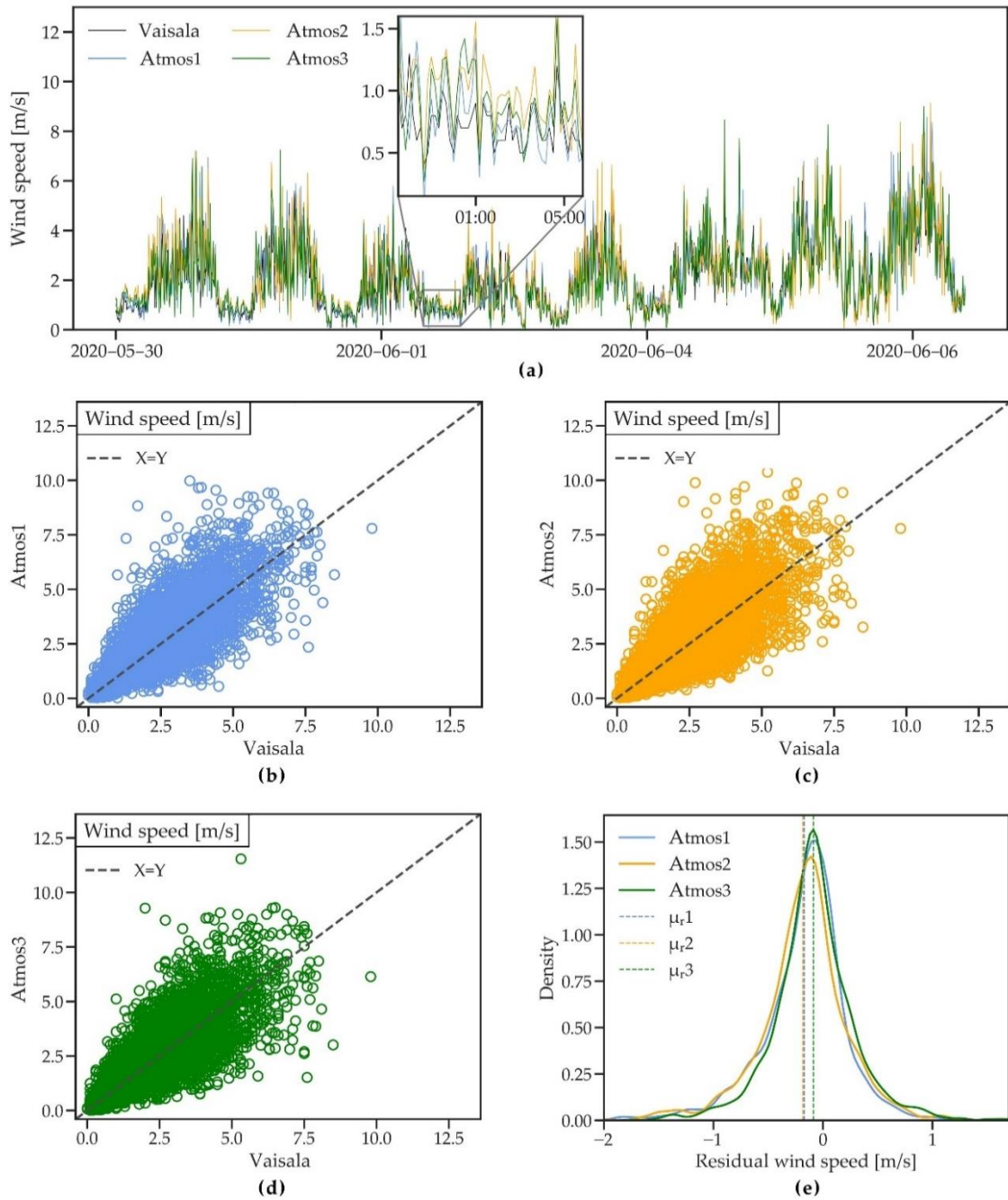


Figure 2.9 (a) A short time series of wind speed measured by three ATMOS41 weather stations and the ICOS-bkp station from 30 May to 6 June 2020. (b–d) Scatterplots of 10 min wind speed for the three ATMOS41 stations vs. the reference station. (e) Probability density functions of the residual mean hourly wind speed. Dashed lines show the mean of residuals ( $\mu_r$ ).

Wind direction was compared by drawing wind roses for each station (Figure 2.10a–d), where the length of the bins represents the frequency of the observed direction in percent, while colours indicate the magnitude of wind speed. West to South-West and East are dominant wind directions that occur, in total,  $\sim 40\%$  of the time with a top frequency of around 7.5% for West/South-West, while wind from the North is observed in total  $\sim 13\%$  of the time. The measurements from the Vaisala station agree well with the commonly

observed wind direction at the Selhausen site [Schmidt *et al.*, 2012]. Strong winds were mainly observed from West and South-West and sometimes from the North, while East winds were considerably weaker. Wind roses from the ATMOS41 stations agree in the main wind directions and speed with the reference station. Atmos1 more frequently recorded northerly winds with a top frequency of  $\sim 7\%$ , while Atmos2 and Atmos3 recorded West/South-West winds with a higher frequency of  $\sim 10\%$  as compared to the reference station. Wind roses for the newer ATMOS41 stations differ somewhat from that of Atmos1 likely due to adjustments made by the manufacturer (Section 2.3.1). Although our results do not show a significant improvement of the measurement from the older Atmos1 (2017 version) to the newer ATMOS41 stations, wind direction is still measured reasonably well by the ATMOS41.

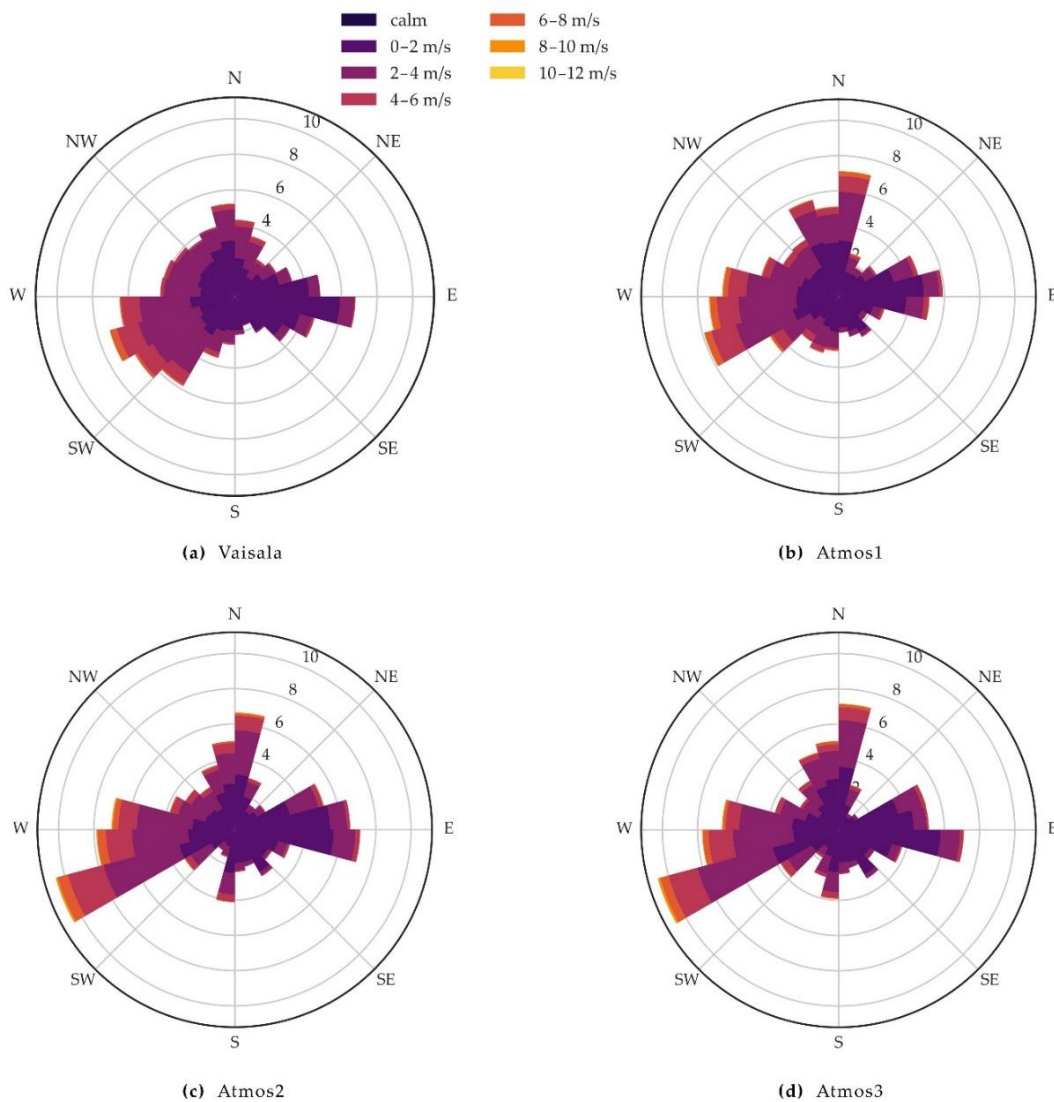


Figure 2.10 Wind roses showing the frequency of observed wind direction at a 10 min interval measured by (a) the Vaisala reference station. (b–d) the three ATMOS41 weather stations, for the period from 23 April to 5 July 2020.



## 2.4 Conclusions

This study evaluated the performance of the ATMOS41 all-in-one weather station over a period of 73 days by assessing the inter-sensor variability of three stations and by comparison against high quality, highly standardized reference meteorological stations. Inter-sensor comparison of the three ATMOS41 stations showed overall close agreement for most variables, while the newer Atmos2 and Atmos3 stations performed better in measuring atmospheric pressure, relative humidity and solar radiation compared to the older Atmos1 (2017 version). Solar radiation showed the greatest improvement, where the bias was reduced from 35.22 W/m<sup>2</sup> to ~9.55 W/m<sup>2</sup>. Generally good agreement with  $R^2 > 0.95$  and small biases were observed for most of the examined weather variables when compared to the reference station. If reference solar radiation data are locally available, a simple linear correction function was proposed to account for the 3% systematic bias that remained in solar radiation measured by the ATMOS41. The atmospheric pressure sensor of the ATMOS41 showed only moderate performance compared to the ICOS station, showing greater uncertainty in the measurements than recommended by the “achievable uncertainty” standard commissioned by the WMO. The measurement of wind speed by the ATMOS41 was slightly overestimated and showed relatively large scatter. Better results are achieved with hourly or half-hourly averages, which are suitable for most modelling applications. The largest variability between the stations was found in the measurement of precipitation, where total precipitation measured by the ATMOS41 showed differences around  $\pm 7.5\%$  compared to the reference. This was attributed mainly to wind-induced errors that may have been exacerbated due to the close proximity of the three ATMOS41 stations as well as differences in the measurement resolution and architecture of the compared rain gauges.

The results of this study showed similar or improved performance of the ATMOS41 compared to the early performance test, but also revealed its limitations. Further work should focus on the performance assessment of the ATMOS41 during extreme precipitation and wind speed as well as the long-term durability and accuracy of the station. The station seems to be well suited for private users. In particular, farmers in high-income countries can benefit from its compact design and limited maintenance requirements. Developing countries may similarly benefit from the ATMOS41 station when costs are jointly carried by multiple actors that use the collected data to market data products to private and governmental institutions. This strategy is applied within the

TAHMO project. Due to the higher uncertainty related to atmospheric pressure and precipitation measurements, and the non-heated gauge, the use of the ATMOS41 station in research appears to be better suited for studies where the amount of solid precipitation is not relevant, where precise rainfall or atmospheric pressure is not a key parameter or when multiple gauges can be deployed to calculate average values for a given location. Overall, the ATMOS41 is a good compromise between measurement accuracy and cost effectiveness, making it an attractive component of wireless sensor networks as well as an expansion tool for weather monitoring networks in remote areas or under limited financial resources.

### 3 **CLM5-FruitTree: A new sub-model for deciduous fruit trees in the Community Land Model (CLM5)**

This chapter is based on the following journal article:

**Dombrowski, O.**, Brogi, C., Hendricks Franssen, H.-J., Zanutelli, D., & Bogen, H. (2022). CLM5-FruitTree: a new sub-model for deciduous fruit trees in the Community Land Model (CLM5). *Geoscientific Model Development*, 15(13), 5167-5193. <https://doi.org/10.5194/gmd-15-5167-2022>

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#### **Abstract**

The inclusion of perennial, woody crops in land surface models (LSMs) is crucial for addressing their role in carbon (C) sequestration, food production, and water requirements under climate change. To help quantify the biogeochemical and biogeophysical processes associated with these agroecosystems, we developed and tested a new sub-model, CLM5-FruitTree, for deciduous fruit orchards within the framework of the Community Land Model version 5 (CLM5). The model development included (1) a new perennial crop phenology description, (2) an adapted C and nitrogen allocation scheme, considering both storage and photosynthetic growth of annual and perennial plant organs, (3) typical management practices associated with fruit orchards, and (4) the parameterization of an apple plant functional type. CLM5-FruitTree was tested using extensive field measurements from an apple orchard in South Tyrol, Italy. Growth and partitioning of biomass to the individual plant components were well represented by CLM5-FruitTree, and average yield was predicted within 2.3% of the observed values despite low simulated inter-annual variability compared to observations. The simulated seasonal course of C, energy, and water fluxes was in good agreement with the eddy covariance (EC) measurements owing to the accurate representation of the prolonged growing season and typical leaf area development of the orchard. We found that gross primary production, net radiation, and latent heat flux were highly correlated ( $r > 0.94$ ) with EC measurements and showed little bias ( $< \pm 5\%$ ). Simulated respiration components, sensible heat, and soil heat flux were less consistent with observations. This was attributed to simplifications in

the orchard structure and to the presence of additional management practices that are not yet represented in CLM5-FruitTree. Finally, the results suggested that the representation of microbial and autotrophic respiration and energy partitioning in complex, discontinuous canopies in CLM5 requires further attention. The new CLM5-FruitTree sub-model improved the representation of agricultural systems in CLM5 and can be used to study land surface processes in fruit orchards at the local, regional, or larger scale.

### 3.1 Introduction

Orchards and other perennial fruit crops are a major component of the global agricultural production with significant coverage and yield in China, the United States, south-western Africa, and some parts of Europe [FAO, 2021a]. In the European region, perennial crops are a key economic element of Mediterranean agro-ecosystems as they provide 45% of the local agricultural output [Lobianco and Roberto, 2006]. Apples are the most important fruit tree crop as one third of European orchards is devoted to their production. With a coverage of 984,509 ha, they provide a yearly harvest of over 17 million tons which is one fifth of the overall European fruit production in terms of output value [FAO, 2021a].

In contrast to annual crops, fruit trees can be productive for several decades before rotation is needed. Their prolonged growing season, standing biomass, and low respiratory losses can support carbon (C) storage and promote higher C use efficiencies [Wiinsche and Lakso, 2000; Zanutelli *et al.*, 2013]. The transport of C stored in biomass into the soil in addition to reduced soil tillage and disturbances under fruit orchards compared to annual crops further promote C sequestration [Bwalya, 2012; Ledo *et al.*, 2020; Wu *et al.*, 2012]. The FAO has therefore suggested perennial agriculture as a possible measure to mitigate climate change and enhance food security [Glover *et al.*, 2010], and many studies have recently investigated this potential for various fruit orchards [Hammad *et al.*, 2020; Scandellari *et al.*, 2016; Wu *et al.*, 2012; Yasin *et al.*, 2021]. The study of water and irrigation requirements in fruit orchards has become another field of intense research due to the need for a more resilient agriculture in the context of climate change and water supply shortages [El Jaouhari *et al.*, 2018; Maestre-Valero *et al.*, 2017; O'Connell and Scalisi, 2019; Segovia-Cardozo *et al.*, 2022]. In order to answer questions related to C sequestration, water requirements, and sustainable food

production of fruit orchards, a better understanding of the related ecosystem processes is vital [Fader *et al.*, 2015].

Models with a comprehensive description of the carbon, water, and energy fluxes, such as global land surface models (LSMs), are a powerful tool to explore complex ecosystems like the abovementioned fruit orchards. The use of LSMs was recently extended to not only model the processes at the land–atmosphere interface, but also to study the response of ecosystems and water resources to climate change [Blyth *et al.*, 2021; Fisher and Koven, 2020; Prentice *et al.*, 2015]. To quantify these effects, LSMs need to represent a wide range of land use and vegetation types. However, most LSMs consider only perennials such as deciduous and coniferous trees, as well as major annual crops such as wheat, soy, or maize [Lawrence *et al.*, 2018]. Recently, some LSMs additionally included bioenergy crops [Schaphoff *et al.*, 2018], while others group crops into a few generic crop types [Balsamo *et al.*, 2009; Krinner *et al.*, 2005; Noilhan and Mahfouf, 1996]. Despite their significance, perennial crops, such as fruit trees, are rarely considered in LSMs and attempts of including them in global and regional modelling environments are scarce [Cheng *et al.*, 2020; Fader *et al.*, 2015]. An example of such an attempt is the inclusion of agricultural trees (e.g., grapes, cotton, and apple trees) in the Lund-Potsdam-Jena managed Land (LPJmL) model to improve the representation of Mediterranean agroecosystems [Fader *et al.*, 2015]. Here, agricultural trees were modelled as small trees and fruit harvest was determined as the product of a plant specific harvest index and the net primary productivity (NPP). Other authors parameterized oil palm trees, a perennial evergreen crop, in the Community Land Model (CLM) version 4.5 [Fan *et al.*, 2015]. Palm trees were represented by a new phenology where large palm leaves with fruit bunches emerge successively, leaves are pruned regularly, and harvest occurs once a month. Recently, two perennial grasses for energy production were parameterized in the latest version of the model, CLM5 [Cheng *et al.*, 2020]. Parameters for bioenergy crops were tuned using sensitivity analysis and observations, while harvest was represented by removing around 70% of the aboveground biomass.

While the abovementioned studies describe some common features of perennial plants, they do not, or only partially, represent the seasonal deciduous phenology of fruit trees or the explicit modelling of fruit growth. Furthermore, key aspects such as C reserve accumulation and mobilization in the following spring are generally not considered, possibly due to necessary simplifications or because the drivers of these processes are

still not fully understood [*Le Roux et al.*, 2001; *Neumann*, 2020]. The absence of perennial crops in land surface models introduces a significant bias in the representation of biogeophysical and biogeochemical processes in agro-ecosystems where this type of cultivation is prevalent. As a result, the response to climate change in terms of C sequestration, water requirements, or food production cannot be assessed adequately in regions such as the Mediterranean, where perennial, woody crops are very common and play a vital role for food security and economy [*Fader et al.*, 2015; *Lobianco and Roberto*, 2006].

Although deciduous fruit trees share certain characteristics with natural vegetation and annual crops in LSMs such as CLM5, several particularities in their growth dynamics and management practices still prevent a meaningful simulation using currently available representations of vegetation. In this study, we therefore provide CLM5 with the ability to model perennial fruit trees and the associated processes. For this purpose, we developed a new sub-model named CLM5-FruitTree within the existing model framework of CLM5. CLM5-FruitTree combines elements of the broadleaf deciduous tree subroutine such as growth and C turnover of woody components, with distinctive phenological stages and a harvestable organ similar to the annual crop subroutine. We first describe the model conceptualization including the new phenology, carbon and nitrogen (CN) allocation, and management options. We further demonstrate the applicability of CLM5-FruitTree by parameterizing a new apple plant functional type (PFT). Finally we evaluate and discuss the model performance using extensive field data from an apple orchard in South Tyrol, Italy.

## **3.2 Methods**

### **3.2.1 Vegetation characterizations in CLM5**

The latest version of the Community Land Model, CLM5, simulates the exchange of water, energy, C, and nitrogen (N) between land and atmosphere as well as their storage and transport on the land surface and in the subsurface, driven by climate variability and modulated by soil and vegetation states and characteristics. The land surface in CLM5 is characterized by one of five land units namely glacier, lake, urban, vegetated, and crop. These units are further divided to capture the variability in soil, vegetation, and

management options (i.e., irrigated or non-irrigated). Compared to previous model versions, CLM5 features various improvements in the representation of land use and vegetation modelling such as plant CN cycling, soil and plant hydrology and crop modelling [Lawrence *et al.*, 2018; Lombardozzi *et al.*, 2020].

Many of the C and N cycle components of CLM5 were originally derived from the Biome BioGeochemical Cycles (Biome-BGC) model [Thornton *et al.*, 2002]. Here, vegetation is represented conceptually by three different plant C and N pools that are maintained separately for the individual plant organs (leaf, live/dead stem, fine root, live/dead coarse root, and grain). The storage pools represent C and N reserves, the transfer pools serve as intermediate pools to separate fluxes in and out of the storage pools, and the display pools represent the actual growth of a given organ (Figure 3.1). C made available through photosynthesis is first used to support maintenance respiration of live organs based on organ N content, temperature, and a constant base rate as proposed by Atkin *et al.* [2015]. Dead stem and dead coarse root components are assumed to consist of dead xylem cells, without metabolic function (no C cost for maintenance). The remaining C can then be allocated to the growth of new tissue considering associated growth respiration costs. Maintenance respiration, growth respiration and C cost of N uptake from the soil comprise the autotrophic respiration component ( $R_a$ ) in CLM5. Plant material reaching the end of its lifespan feeds into different litter pools from where it progressively decomposes to soil organic matter under C losses through heterotrophic respiration ( $R_h$ ).

For the simulation of fruit orchards, a module for perennial deciduous crops is needed which is currently missing in CLM5. Such a module must account for the perennial deciduous nature of fruit trees, which is similar to the existing representation of broadleaf deciduous trees (BDTs) included in Biome-BGC but with differences in phenological triggers, vegetation structure, and C partitioning. In addition, it must represent growth and harvest of the fruits and typical management practices, of which some are already conceptualized in the prognostic Biogeochemistry Crop Module (BGC-crop), while others are not yet implemented. The algorithm for the seasonal phenology of BDT controls initial leaf development and senescence that mark the beginning and end of a growing season based on temperature and day length thresholds. Once a new growth period is initiated, C and corresponding N fluxes accumulated in the previous season, occur out of the storage pools into the transfer pools, from where they are gradually sent to the display pools (Figure 3.1). During the active growth period, C and corresponding

N storage pools are replenished based on specified C:N ratios of each plant organ. During leaf senescence, C and N pools feed the litter or coarse woody debris pool except for live stem and live coarse roots that are mostly retained as structural woody tissue (dead stem and dead coarse roots).

BGC-crop, adopted from the prognostic crop module of the Agro-Ecosystem Integrated Biosphere Simulator (Agro-IBIS), currently features eight different annual crop species with interactive crop management options (i.e., irrigation and fertilization). Another 23 currently inactive crop types can be defined but have not been provided with specific crop parameters [Lombardozzi *et al.*, 2020]. Crop phenology and CN allocation follow three phenological phases: (1) from planting to leaf emergence, (2) from leaf emergence to the start of grain fill, and (3) from grain fill to grain maturity and harvest, which are controlled by temperature and growing degree-day (GDD) thresholds. Different to natural vegetation, crops have a grain pool representing the harvestable organ but no structural woody tissue. Furthermore, all assimilates are directed to the displayed pools while the storage pools remain unused. At harvest, C and N from the grain pool are transferred to a grain product pool while a small amount is kept to reseed the crop in the following year. All remaining plant parts feed the litter cycle (Figure 3.1). The reader is referred to Lombardozzi *et al.* [2020] and the technical documentation of CLM5 for a more detailed description of the BDT and crop representation [Lawrence *et al.*, 2018].

From the above description of the existing vegetation modules, the following limitations for the application of CLM5 to deciduous fruit trees arise. (1) The current BGC-crop algorithm does not allow the simulation of perennial and/or woody crops. (2) The BDT phenology algorithm although describing some characteristics common to fruit trees, lacks the capability to simulate a harvestable organ, individual development of different plant parts, and the separation of growth from C reserves of the previous year and photosynthetic growth of the current season. (3) Typical management practices of fruit orchards such as transplanting of tree seedlings and pruning are currently not represented in CLM5. (4) There is no parameterized fruit tree PFT in the default parameter set of CLM5.

### **3.2.2 Model conceptualization and technical implementation**

To resolve the model limitations discussed in Section 3.2.1, we developed a new sub-model CLM5-FruitTree to model the ecosystem processes and exchanges of energy and



matter of deciduous fruit trees grown in commercial orchards with a focus on the simulation of biomass growth and yield. More specifically, for the implementation of CLM5-FruitTree, we introduced a new phenology subroutine that describes the main phenological development of fruit trees and includes triggers for seasonal orchard management practices typical under organic or conventional production. In addition, the CN allocation module as well as corresponding modules (C and N state and flux updates) were modified to reproduce the growth dynamics of fruit trees and to model the fates of C and N in the orchard system. The sub-model development does not include any changes to the existing calculation schemes for radiative transfer or momentum, heat, and water fluxes to explicitly account for the discontinuous canopy structure of tree rows and vegetated or non-vegetated alleys in fruit orchards. In-row and between-row planting distances and alley vegetation are not defined directly. Instead, the orchard structure and the area covered by the canopy are accounted for through parameterization of the leaf and stem area indices, the planting density, maximum canopy height, and aerodynamic parameters, similar to the implementation of crops and forest in CLM5.

CLM5-FruitTree combines characteristics of both BDT and annual crops to simulate a perennial woody crop with a harvestable organ making use of the existing concepts of storage, transfer, and display vegetation pools described in Section 3.2.1 (Figure 3.1). Similar to the existing BDT phenology algorithm in CLM5, the fruit tree algorithm uses a perennial deciduous phenology with standing woody biomass and annual leaf shedding. During the active growth period however, the phenology and CN allocation of vegetative and harvestable organs are described by distinct growth phases and are driven by a GDD summation similar to the crop phenology.

An orchard is established by transplanting small tree seedlings from a nursery, a typical planting method for this type of cultivation [Corelli-Grappadelli and Marini, 2008; Wheaton *et al.*, 1990]. Once planted, the orchard remains productive according to a user-defined lifespan which, depending on fruit tree type and production system, typically ranges between 10 and 30 years [Cerutti *et al.*, 2014; Demestihis *et al.*, 2017]. The sub-model makes no specific assumptions about the rootstock, but the effect of different rootstocks in terms of tree height and rooting depth can be set by the user via the respective parameters,  $z_{topmx}$  and  $root\_dmx$  (Table A.2). In CLM5-FruitTree, both stored C and current photosynthesis contribute to the growth of the fruit tree, as leaf and shoot development at the beginning of a growing season utilizes carbohydrate reserves and

nitrogenous compounds that were accumulated during the previous season [Loescher *et al.*, 1990; Oliveira and Priestley, 1988; Tromp, 1983]. Deciduous fruit trees are dormant in winter and resume growth in spring after meeting species- and cultivar-specific chilling and heat requirements [Anderson *et al.*, 1985; Faust *et al.*, 1997; Zavalloni *et al.*, 2006], which is represented in CLM5-FruitTree using the chilling and forcing model proposed by Cesaraccio *et al.* [2004]. Early in the season, the canopy develops rapidly until it reaches maturity typically by midsummer, while leaf shedding occurs when temperatures drop in autumn [Kozłowski, 1992; Lakso *et al.*, 1999; Loescher *et al.*, 1990]. Fruit trees usually start flowering 3–4 weeks after bud break, which is not specifically represented by CLM5-FruitTree which instead assumes that fruit growth begins at the end of flowering [Lakso *et al.*, 1999]. The implementation of flowering to include effects of non-optimal pollination, frost during flowering, or hormonal processes affecting fruit set and development is outside of the scope of this development and of minor importance for large-scale simulations and processes at ecosystem level that are typically the focus of LSMs such as CLM5. Consequently, CLM5-FruitTree does not produce information on fruit size or number but only on total yield which we consider adequate for most applications of the sub-model development. Fruit growth is described by two stages, cell division and cell expansion that together form a sigmoid growth curve observed for many fruit tree species such as apple, pear, and orange [Corelli-Grappadelli and Lakso, 2002; Jackson, 2011].

In the following, the new developments to account for the distinct phenology, CN allocation, and management practices of a fruit orchard are described in more detail. Other biochemical and biophysical processes such as photosynthesis, water and litter cycles, and fixation and uptake of N were not modified except for minor adaptations to the re-translocation of N and respiration to enable the use of certain parts of these scripts for the fruit tree PFT. The technical implementation of some features of the new phenology routine (transplanting, pruning, harvest, and final rotation) was based on CLM-Palm, a previous model development for palm trees in CLM4.5 (Fan *et al.* [2015] and unpublished code). References where code elements were directly reused or modified based on CLM-Palm are made in the published source code of CLM5-FruitTree [Dombrowski, 2022]. Along with the new sub-model, an apple PFT was parameterized using one of the existing but thus far inactive crop types in CLM5, types 35 and 36 (rainfed and irrigated citrus).

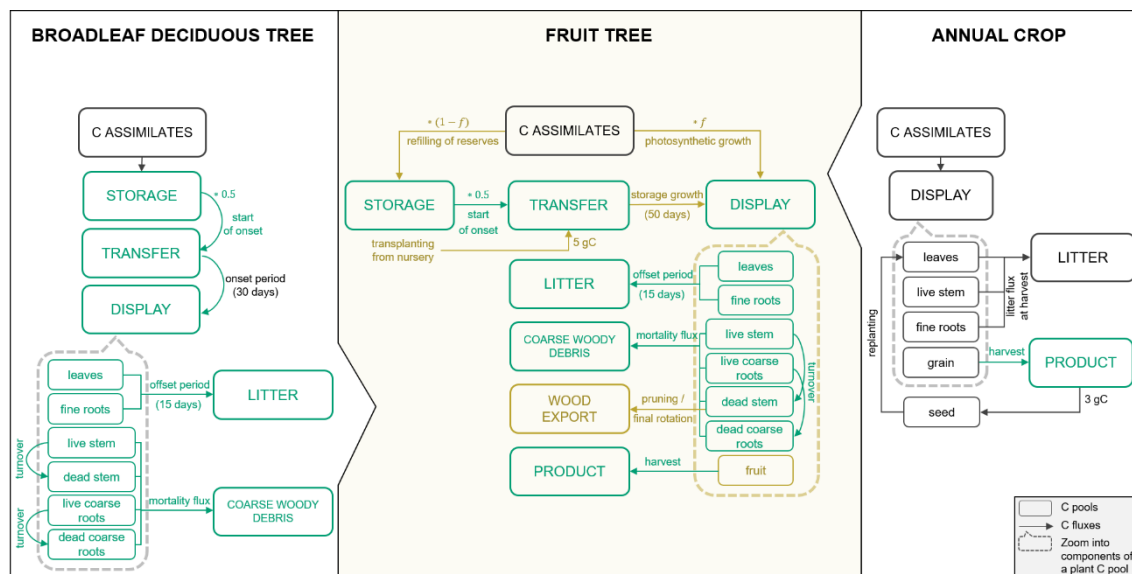


Figure 3.1 Schematic of the main phenology and C allocation features of the broadleaf deciduous tree and annual crop representations in CLM5 as well as the new sub-model CLM5-FruitTree. C pools within the dashed boxes are the individual components that make up the displayed C pool (the same components can be found for the other main plant pools: storage and transfer pools respectively). Carbon pools and fluxes in green were reused for CLM5-FruitTree while pools and fluxes in brown were modified or newly added.

### 3.2.2.1 Phenology

A new orchard life cycle is initialized by transplanting seedlings at the beginning of the year during dormancy. Tree growth thereafter is described by six post-planting phenological stages, namely: (1) bud break, (2) fruit growth, (3) fruit ripening, (4) canopy maturity, (5) fruit maturity and harvest, and (6) start of leaf senescence (Figure 3.2).

Bud break is predicted by a sequential model that first accumulates chill days followed by anti-chill days based on a predefined temperature threshold and chilling requirement [Cesaraccio *et al.*, 2004]. More information on the sequential model and the calibration of model parameters can be found in Appendix III. Outside the dormant period, leaf and fruit development occurs in parallel but with a time shift as fruit growth typically starts 4–5 weeks after bud break while canopy development continues until mid-season and leaf senescence does not occur until after the fruits are harvested [Goldschmidt and Lakso, 2005; Wünsche and Lakso, 2000] (Figure 3.2).

The thermal thresholds to reach phases (2)–(5) are defined as accumulated GDDs since bud break and can be adjusted by the user via the parameter file which applies to all parameters listed in Table A.2 of the Appendix. GDDs are determined as the difference between the average daily air temperature and a base temperature of 4 °C with a maximum daily increment of 26 degree days (Eq. (3.1)). Different to the existing deciduous phenology, leaf senescence is triggered not by day length but by the drop of the daily

mean temperature below a critical temperature threshold, in this case the base temperature. This approach was selected since many fruit trees that belong to the Rosaceae family (e.g., apple, pear, plum, and cherry) are unaffected by photoperiod and instead controlled by temperature [Heide and Prestrud, 2005]. The last day of the leaf senescence period marks the beginning of dormancy. The new phenology subroutine of CLM5-FruitTree also controls C reserve dynamics, stem and root turnover, and final rotation, which involves removing and replanting trees when the maximum orchard lifespan is reached.

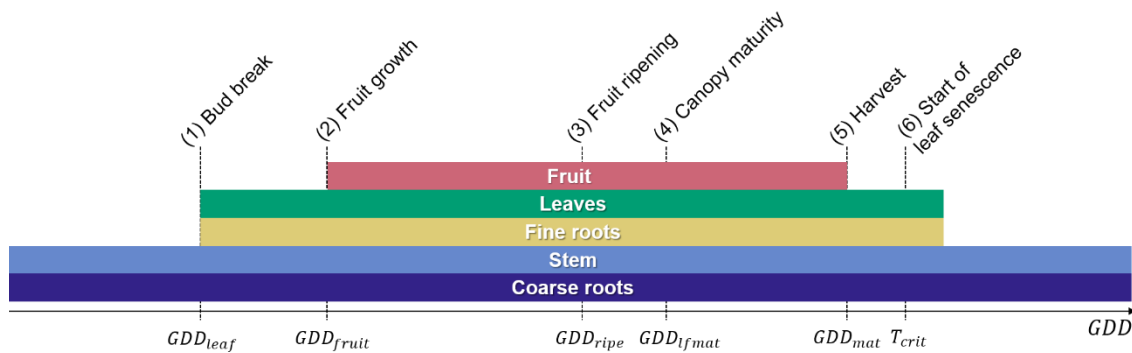


Figure 3.2 Fruit tree phenological stages of (1) bud break at the end of dormancy, (2) the start of fruit growth, (3) fruit ripening, (4) canopy maturity, (5) harvest, and (6) the start of leaf senescence. The lengths of phenological stages (2)-(5) are determined by their respective growing degree-day thresholds (GDD) starting from bud break ( $GDD_{leaf}=0$ ), while stage (6) is determined by a critical temperature threshold ( $T_{crit}$ ). Coloured bars correspond to the time any plant organ is present on the field throughout a year.

### 3.2.2.2 Carbon and nitrogen allocation

CN allocation to the growth of new tissue (display pools) and to storage pools follows the phenological stages described in Section 3.2.2.1 (Figure 3.2). A coupled CN allocation subroutine determines the fate of newly assimilated C from photosynthesis. A user-defined initial biomass can be assigned to leaf and fine root transfer pools via the *transplant* parameter (Table A.2), while additionally 10% of this biomass is assigned to the dead stem pool to define an initial stem area index  $> 0$ . Each pool is also assigned the corresponding amount of N. Adjustments to this parameter have only little effect on the biomass growth and yield of the adult trees as the trees reach their maximum canopy height and develop their full leaf area index (LAI) within the first couple of years after transplanting. Thereafter, the potential allocation to the different plant components is based on allocation coefficients and allometric relationships between dead and live parts of stem and coarse root. Throughout the growing period until harvest, 5% of the newly assimilated C is allocated to the storage pools, as defined by the *fcur* parameter, except for fruits where all allocated C is assigned to the displayed pool. For all other organs, the

remaining C is also allocated to the displayed C pools. At bud break, a fraction of the C in the storage pool of all plant components, except fruits, is transferred to the actively growing C pools over a period that can be specified by the newly added parameter  $ndays_{stor}$ . This is based on the assumption that resources are partially mobilized to support growth of new tissue [Loescher *et al.*, 1990; Oliveira and Priestley, 1988]. Lacking more specific knowledge of the exact fraction, the default of 0.5 used by the seasonal deciduous phenology in CLM5 is adopted for fruit trees.

Before the start of fruit growth, phase (1), newly assimilated C and corresponding N are partitioned between leaf, stem, and root pools. The allocation coefficients are calculated according to a set of equations that were adapted from the AgroIBIS crop phenology algorithm used in CLM5-BGC-crop [Lawrence *et al.*, 2018]:

$$GDD_{T_{2m}} = GDD_{T_{2m}} + T_{2m} - T_f - 4 \quad \text{where} \quad 0 \leq T_{2m} - T_f - 4 \leq 26 \text{ } ^\circ\text{days}, \quad (3.1)$$

$$a_{repr} = 0, \quad (3.2)$$

$$a_{froot} = a_{froot}^i - (a_{froot}^i - a_{froot}^f) * \frac{GDD_{T_{2m}} - GDD_{leaf}}{GDD_{fruit} - GDD_{leaf}}, \quad (3.3)$$

$$a_{leaf} = (1 - a_{froot}) * \frac{a_{leaf}^i * (e^{-b} - e^{-b * \frac{GDD_{T_{2m}} - GDD_{leaf}}{GDD_{lfmat} - GDD_{leaf}}})}{e^{-b} - 1}, \quad (3.4)$$

$$a_{livestem} = 1 - a_{repr} - a_{froot} - a_{leaf}, \quad (3.5)$$

where  $GDD_{T_{2m}}$  are the accumulated growing degree days for the 2 m air temperature with maximum increments of 26 degree days;  $T_{2m}$  is the simulated 2 m air temperature in K;  $T_f$  is the freezing temperature of water and equals 273.15 K;  $GDD_{leaf}$ ,  $GDD_{fruit}$ , and  $GDD_{lfmat}$  are thermal thresholds for bud break, start of fruit growth, and canopy maturity, respectively;  $b$  is an exponential factor;  $a_{leaf}^i$ ,  $a_{froot}^i$ , and  $a_{froot}^f$  are initial and final values for the allocation coefficients to leaf ( $a_{leaf}$ ) and fine root ( $a_{froot}$ ), respectively; and  $a_{repr}$  and  $a_{livestem}$  are the allocation coefficients to fruit and live stem, respectively.

Once fruit growth begins in phase (2), an increasing proportion of the assimilated C and corresponding N is allocated to this organ, causing leaf allocation to decline and fruit

allocation to plateau at a high value once canopy maturity is reached. Allocation to fine roots and stem continues to decline and then settles at a constant value until harvest:

$$a_{livestem} = a_{livestem} * \left( 1 - \frac{(GDD_{T2m} - GDD_{leaf}) - (GDD_{fruit} - GDD_{leaf})}{(GDD_{mat} - GDD_{leaf})^{d_L - (GDD_{fruit} - GDD_{leaf})}} \right)^{d_{alloc}^{stem}}, \quad (3.6)$$

$$a_{repr} = 1 - a_{froot} - a_{livestem} - a_{leaf}, \quad (3.7)$$

where  $GDD_{mat}$  is the thermal threshold for fruit maturity and harvest, while  $d_L$  and  $d_{alloc}^{stem}$  are stem allocation decline factors.

After harvest and until the start of dormancy, all of the newly assimilated C is sent to the storage pools following the notion that late in the season, assimilates are used mostly to fill up reserves that can be mobilized to resume growth in the following spring [Le Roux *et al.*, 2001]. Fruit trees store C in the perennial woody parts of the tree, from where it is re-mobilized to support the growth of new shoots, leaves, and fine roots [Le Roux *et al.*, 2001; Millard, 1996; Oliveira and Priestley, 1988]. Since in CLM5 separate storage pools are assigned to each plant organ, the newly added *aleafstor* parameter (Table A.2) defines the fraction of allocatable C going to the leaf storage pool, while the remainder is split equally between roots and stem.

Fruit trees, similar to other deciduous species, have been observed to translocate N out of senescent leaves to be reused by other tree organs [Malaguti *et al.*, 2001; Millard, 1996; Millard *et al.*, 2006]. Therefore, CLM5-FruitTree adopts the same N re-translocation strategy as used in the BDT phenology during which N is removed from falling litter based on leaf and litter C:N ratios and the available C to pay for the extraction of N from increasingly recalcitrant litter pools. Subsequently it is transferred to the plant N pool from where it can be used for the growth of new plant tissue [Lawrence *et al.*, 2018].

### 3.2.2.3 Representation of management practices

Furthermore, management practices such as fertilization and stem pruning are represented in the new sub-model. Fertilization is performed on a yearly basis after the occurrence of bud break, as N fertilization in early spring is still the most common practice in fruit orchards even though autumn fertilization or multiple applications via fertigation are also in use to increase fertilizer N use efficiency and reduce N losses [Carranca *et al.*, 2018; Sanchez *et al.*, 1995]. We use the existing fertilization scheme of the crop phenology that

adds fertilizer directly to the soil mineral N pool. A user-defined fertilization rate or amount can be applied as synthetic fertilizer or manure respectively, although there currently is no difference in model behaviour for these two fertilizer types [Lawrence *et al.*, 2018].

Winter pruning is a common practice in fruit orchards and may be performed throughout the winter to control the shape and size of fruit trees, and partially to manage crop load [Grechi *et al.*, 2008]. In many intensive orchard production systems, pruning residues are mulched into the soil, possibly increasing C sequestration [Aguilera *et al.*, 2015; Montanaro *et al.*, 2010]. Alternatively, residues may also be exported and treated as waste [Benyei *et al.*, 2018] or utilized for energy production [Kazimierski *et al.*, 2021]. In CLM5-FruitTree, pruning is performed as the tree enters dormancy by removing a user-defined fraction, *prune\_fr* (Table A.2), of the dead stem from both storage and displayed C pools. We remove C from the dead stem pool instead of the live stem pool since the former is the main wood pool in CLM5 that receives 85% of the C allocated to total new wood. Furthermore, the implemented live wood turnover in CLM5 converts live stem to dead stem at the end of the growing season to account for differences in maintenance respiration and C:N ratios between these tissue types [Lawrence *et al.*, 2018]. Hence the live stem C pool remains rather small and stable over the years, so that applying pruning to this pool would have little effect on total tree biomass. The pruning implemented in CLM5-FruitTree affects only the tree biomass and height that are calculated based on this biomass pool, which in turn affects the calculation of turbulent fluxes of sensible and latent heat. However, this effect is small, and since turbulent fluxes are generally low in winter, the exact timing of pruning does not play a significant role in the magnitudes of these fluxes. During the first three years after planting, trees are not pruned to allow some initial stem biomass to grow. The sub-model treats pruning residues in one of two ways to account for their possible difference in fate: (1) residues are added to the wood harvest pool and exported from the field or (2) residues are added to the woody debris pool thus feeding the litter cycle.

When the orchard reaches the end of its lifespan, C of all biomass pools (storage, transfer, and display) is sent to either the litter pool for leaves and fine roots, or the wood harvest pool for live and dead stem and coarse roots, while any remaining C in the fruit pool is harvested. The orchard can then be replanted in the following year. Lastly, the standard

irrigation routine implemented in CLM5 can be used for irrigated orchards by selecting the irrigated crop PFT.

### 3.2.3 Model implementation and testing

#### 3.2.3.1 Site data

Extensive field measurements from an apple-growing region in the Adige River valley, South Tyrol, Italy (46°21' N, 11°16' E; 240 m a.s.l.) were used to parameterize and test the new CLM5-FruitTree sub-model along with the new apple PFT [Zanotelli *et al.*, 2019; Zanotelli *et al.*, 2015; Zanotelli *et al.*, 2013]. Measurements were obtained from an approximately 0.5 ha irrigated apple orchard planted in 2000 with the Fuji apple cultivar grafted on M9 dwarfing rootstock. The apple trees were planted at a row and tree spacing of 3x1 m (3333 trees per hectare). A 1.8 m wide grass strip was grown between the tree rows, which was mowed three times a year. Other management practices included regular pruning, spring fertilization of 7.5 gN m<sup>-2</sup> yr<sup>-1</sup>, and tillage of the soil directly underneath the trees [Zanotelli *et al.*, 2013]. Stand-related data included general stand characteristics and phenology observations, LAI, C:N ratios, rooting distribution at three depth ranges (0–20, 20–40, and 40–60 cm), measurements of the biomass growth of different tree organs at a monthly or seasonal interval, and fruit harvest information (Table 3.1). Furthermore, daily soil respiration measurements from a control and a trenching plot (with (R<sub>s</sub>) and without (R<sub>h</sub>) root respiration, respectively) were performed in 2010. Additionally, an eddy covariance (EC) station provided measurements of the turbulent exchange of trace gases and energy at the studied apple orchard between 2013 and 2015. The quality check, gap filling, and flux partitioning of collected data followed the procedure outlined in Reichstein *et al.* [2005]. The average closure of the energy balance was 60%. To correct for the closure failure, the missing energy was assigned to the latent (LE) and sensible (H) heat fluxes based on the daily Bowen ratio [Zanotelli *et al.*, 2019]. Measured or derived fluxes included net ecosystem CO<sub>2</sub> exchange (NEE), ecosystem respiration (R<sub>eco</sub>), gross primary production (GPP), LE, H, and evapotranspiration (ET) at half-hourly intervals. Furthermore, soil heat flux (G) measured at 5cm depth as well as soil moisture (SM) measurements up to a depth of 60 cm of soil are available. Table 3.1 gives a summary of the available data and measurement periods. A complete description of the measurement procedures and instruments can be found in Zanotelli *et al.* [2013], Zanotelli *et al.* [2015], and Zanotelli *et al.* [2019].



Meteorological data, recorded partly at the EC tower and at the Laimburg meteorological station located 4 km from the site (46°23' N, 11°17' E; 224 m a.s.l.), were used at an hourly time step to force the model. Measured data included precipitation, solar radiation, net radiation ( $R_n$ , only at the EC tower), air temperature, air pressure (only at Laimburg), relative humidity, and wind speed. Measurements of incoming longwave radiation ( $LW_{in}$ ) were available for 2010 only, but additional calculations following *Konzelmann et al.* [1994] and *Sedlar and Hock* [2009] were produced and used as forcing for the remaining years 2011–2019 (Appendix IV). This was necessary since the use of the internally calculated  $LW_{in}$  in CLM5 resulted in unrealistic underestimations compared to the available measurements of  $LW_{in}$  leading to a significant bias in  $R_n$ .

Table 3.1 Summary of available data from an apple orchard in the Adige River valley, South Tyrol, Italy between 2010 and 2019. Solid lines represent continuous and dotted lines monthly measurements, while diamonds represent single measurements.

| Data   | 2010           | 2011 | 2012 | 2013  | 2014 | 2015 | 2016 | 2017 | 2018 | 2019 |
|--|----------------|------|------|-------|------|------|------|------|------|------|
| Weather data EC tower  | —————          |      |      | ————— |      |      |      |      |      |      |
| Weather data Laimburg  | —————          |      |      |       |      |      |      |      |      |      |
| Biomass (NPP) components   | •••••          | ◆    | ◆    |       |      |      |      |      |      |      |
| C:N ratios of biomass components   | •••••          |      |      |       |      |      |      |      |      |      |
| Leaf area index (LAI)  | •••••••••••••• |      |      |       |      |      |      |      |      |      |
| Fruit production (yield)   |                | ◆    | ◆    | ◆     | ◆    | ◆    | ◆    |      |      |      |
| Root distribution (0-60 cm)  | ◆              |      |      |       |      |      |      |      |      |      |
| Soil respiration ( $R_s$ , $R_h$ )   | —————          |      |      |       |      |      |      |      |      |      |
| Soil heat flux (G)   |                |      |      | ————— |      |      |      |      |      |      |
| Soil moisture (SM, 0-60 cm)  |                |      |      | ————— |      |      |      |      |      |      |
| EC data: carbon (GPP, $R_{eco}$ , NEE),<br>energy ( $R_n$ , LE, H), water (ET) |                |      |      | ————— |      |      |      |      |      |      |

### 3.2.3.2 Model set-up

The model was set up in point mode to simulate the apple orchard in the Adige valley using available sand, clay, and organic matter fractions. The model was spun-up for 200 years, first in accelerated decomposition and then in normal decomposition mode, until all state variables, such as total ecosystem soil C and soil water, reached equilibrium

[Lawrence *et al.*, 2018]. For the model spin-up, the CRUNCEPv7 atmospheric forcing data set from 1986 to 2016 was used [Viovy, 2018]. The apple orchard was then initiated using the newly developed sub-model and the apple PFT selecting the site-specific management (i.e., fertilization with  $7.5 \text{ gN m}^{-2} \text{ yr}^{-1}$ , irrigation, mulching of pruning material). Simulations were performed for a period of 10 years to mirror the time from orchard establishment in 2000 up to the start of the measurements in 2010 using 10 years (2010–2019) of the available meteorological data from Laimburg meteorological station. Simulations were then extended for another 6 years from 2010 to 2015 for model parameterization and performance evaluation purposes.

### 3.2.3.3 Parameterization

Key parameters of the new sub-model as well as other PFT-specific parameters were parameterized using the first 3 years of simulations between 2010 and 2012. The lengths of phenological stages and associated parameters were determined based on field observations of bud break, full bloom, and harvest as well as non-cultivar specific apple phenology descriptions that were found in the literature (Appendix V). The length of the period where growth is supported out of reserves (*ndays\_stor*) was calibrated based on the biomass measurements and the estimate by Zanutelli *et al.* [2013] that apple trees use stored carbohydrates in the first two months after bud break. C allocation coefficients were calculated based on the monthly measurements in 2010 by dividing the biomass growth of the individual plant organs by the total biomass increment. Subsequently, model parameters associated with the CN allocation subroutine (Eq. (3.2) – (3,7)) were calibrated manually to match the coefficients obtained from the observations and the overall biomass partitioning on a yearly basis. Parameter values for C:N ratios of all plant organs and maximum LAI were based on field observations in 2010 and 2010–2012, respectively. The specific leaf area (*slatop*) was calculated by dividing monthly measurements of LAI by leaf biomass and taking the average of the obtained values. Structural and morphological parameters such as maximum tree height (*ztopmx*), planting density (*nstem*), the ratio of stem height to radius at breast height (*taper*), or rooting depth (*root\_dmx*) were adjusted based on site-specific information [Zanutelli *et al.*, 2013]. Initial biomass at transplanting was assumed  $5 \text{ gC m}^{-2}$ , resulting in an initial tree height of around 100 cm and a stem diameter of 16 mm. As seedlings are dormant at the time of transplanting, their LAI is 0. The CLM5 root distribution parameter (*rootprof\_beta*), which sets the root ratios at different depths, was calibrated by least squares regression of

the measured root ratios at 0–20, 20–40, and 40–60 cm depths and the calculated ratios. Optical parameters for leaf transmittance and reflectance in the visible and near-infrared (IR) were set to average values reported for apple by *Bastías and Corelli-Grappadelli* [2012]. Stem reflectance and transmittance were assumed to be similar to other woody species and therefore set to the values used for BDT in CLM5, similar to the assumptions made by *Fan et al.* [2015] for the palm tree development in CLM4.5. The ratio of momentum roughness length to canopy top height ( $z_{0mr}$ ) was set to the average value of the ranges reported for apple and citrus orchards to account for the differences in canopy structure compared to annual crops and forest [*la Fuente-Sáiz et al.*, 2017; *Tanny and Cohen*, 2003]. No specific values could be found for the ratio of displacement to top of canopy height ( $displar$ ), the leaf orientation index ( $xl$ ), or the intercept to calculate the top of canopy maintenance respiration base rate ( $lmr\_intercept\_atkin$ ). These values were assumed to be comparable to other deciduous trees and thus set to the values used for BDT in CLM5. Parameters related to C reserve dynamics (e.g.,  $fcur$ ) and photosynthesis (e.g., the slope of the relationship between leaf N per unit area and the maximum rate of carboxylation at 25 °C,  $s\_vcad$ ) were adjusted to match observed LAI and productivity data. All parameters with their values and references to the literature are summarized in Table A.2 of the Appendix.

#### 3.2.3.4 Sensitivity analysis

A simple one-by-one sensitivity analysis was performed to further tune model parameters and assess the influence of newly added parameters on the simulation results. As a complete sensitivity analysis of all PFT-related parameters would have exceeded the scope of this study, the analysis focused on key parameters of the new phenology and CN allocation subroutines. Other potentially influential parameters were selected based on previously performed sensitivity analyses by *Göhler et al.* [2013] for CLM3.5, and by *Cheng et al.* [2020] and *Dagon et al.* [2020] for CLM5, taking into account differences between previous and current model versions. Parameters selected for the analysis were perturbed by varying a parameter by  $\pm 30\%$ ,  $\pm 20\%$ , and  $\pm 10\%$  while keeping the others fixed to the value of the control simulation (after initial parameterization). The goal here was not to perform an in-depth analysis covering the full range of possible parameter values, but rather to provide a first indication of influential parameters in the new sub-model similar to the approach of *Fan et al.* [2015]. As a measure of sensitivity, the parameter effect (PE) was calculated using the average of three years of simulations

between 2013 and 2015 of the control and the perturbed simulations for selected output variables and the following formula adjusted from *Luo et al.* [2020]:

$$\Delta X_{i,j} = \sum_{k=1}^n \frac{|\overline{X_{i,j,k}} - \overline{X_{i,control}}|}{|\overline{X_{i,control}}|}, \quad (3.8)$$

$$PE_{i,j} = \frac{\Delta X_{i,j}}{\max[(\Delta X_{i,j})_{1 \leq i \leq n; 1 \leq j \leq m}]}, \quad (3.9)$$

where  $X$  is a simulated value of the control or a perturbation run,  $\Delta X$  is the summed absolute difference between the control and the perturbation run across all perturbations,  $k$  is the parameter perturbation factor,  $i$  is the  $i^{\text{th}}$  variable across  $n = 6$  selected output variables including: GPP, NEE,  $R_a$ , LE, maximum LAI, and yield, and  $j$  is the  $j^{\text{th}}$  parameter across  $m$  selected parameters.  $PE_{i,j}$  is a number between 0 and 1 that represents the sensitivity of an output variable  $i$  to the parameter  $j$ , with 1 meaning high and 0 meaning low sensitivity. The parameters selected for sensitivity analysis are indicated in Table A.2 of the Appendix.

### 3.2.3.5 Model performance evaluation

Modelling results are compared to observed biomass, yield, and LAI data as well as ecosystem fluxes retrieved from the EC measurements. Statistical indices for model performance evaluation include the Pearson coefficient of correlation ( $r$ ), the root mean square error (RMSE) and the percent bias (%bias):

$$r = \frac{(\frac{1}{n} \sum_{i=1}^n (X_i^o - \mu^o) * (X_i - \mu))}{\sigma * \sigma^o}, \quad (3.10)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (X_i - X_i^o)^2}, \quad (3.11)$$

$$\%bias = \frac{\sum_{i=1}^n (X_i - X_i^o)}{\sum_{i=1}^n (X_i^o)}, \quad (3.12)$$

where  $i$  is the time step,  $n$  is the total number of time steps, and  $X_i$  and  $X_i^o$  are simulated and observed values at each time step respectively,  $\mu$  and  $\mu^o$  are simulated and observed mean values, respectively, and  $\sigma$  and  $\sigma^o$  are simulated and observed standard deviations.

### 3.3 Results and Discussion

#### 3.3.1 Sensitivity analysis

A total of 34 parameters were initially considered for the sensitivity analysis of which the 13 most influential parameters ( $PE > 0.1$  for at least one of the selected output variables) are shown in Figure 3.3. GPP, NEE,  $R_a$ , and yield have similar sensitivity patterns and are most sensitive to the leaf C:N ratio (*leafcn*) and the relationship between leaf N and the maximum rate of carboxylation at 25 °C (*s\_vcad*). Together with *slatop* and other constants, they control the maximum photosynthetic capacity in the photosynthesis calculation and thus largely influence total C assimilation. As expected, LAI is most influenced by parameters that control the CN allocation to leaves such as the initial leaf allocation coefficient (*fleafi*), the GDDs needed to reach canopy maturity (*lfmat*), the maximum LAI (*laimx*), photosynthetic parameters, and, to a smaller extent, the fraction of C allocated to the leaf storage pool to refill C reserves (*aleafstor*). The first three parameters influence leaf biomass and thus show a considerable effect on GPP, NEE,  $R_a$ , and yield. The same output variables are affected in a similar fashion by the GDDs needed until fruit harvest (*hybgdd*) that control the amount of C allocated to fruits. LE is influenced largely by the parameter controlling stomatal conductance (*medlynslope*), and the photosynthetic parameters (*leafcn*, *s\_vcad*).

Overall, photosynthetic parameters play a key role in determining the magnitude of the studied output variables with an average PE value close to 0.7 across all six variables. Phenological parameters (top seven parameters in Figure 3.3) are generally less influential for the same output variables with average PE values up to 0.43. These findings are largely consistent with earlier studies of parameter sensitivity [Cheng *et al.*, 2020; Dagon *et al.*, 2020; Göhler *et al.*, 2013; Luo *et al.*, 2020]. In contrast to Luo *et al.* [2020], we did not find a strong effect of the root distribution parameter (*rootprof\_beta*) on LE, which can be attributed to the low water stress due to the irrigation management of the studied orchard.

While the one-at-a-time sensitivity analysis provides some insight into model sensitivity, the ranking of influential parameters is strongly influenced by the choice of parameters and output variables, the parameter perturbation strategy (i.e. percent change, linear sampling), and the index chosen as the sensitivity measure. Parameter tuning based on this analysis is further complicated since this approach does not consider parameter covariation that is particularly strong for plant parameters that influence photosynthesis [Göhler *et al.*, 2013]. Selecting parameter values based on the individual best simulation hence does not necessarily yield the best overall result [Luo *et al.*, 2020]. We therefore decided to first adjust  $s\_vcad$  to best match the observed average GPP. In the following, we further adjusted  $fleafi$ ,  $hybgdd$  and  $medlynslope$  to improve the simulated biomass components as well as the LE flux, respectively.

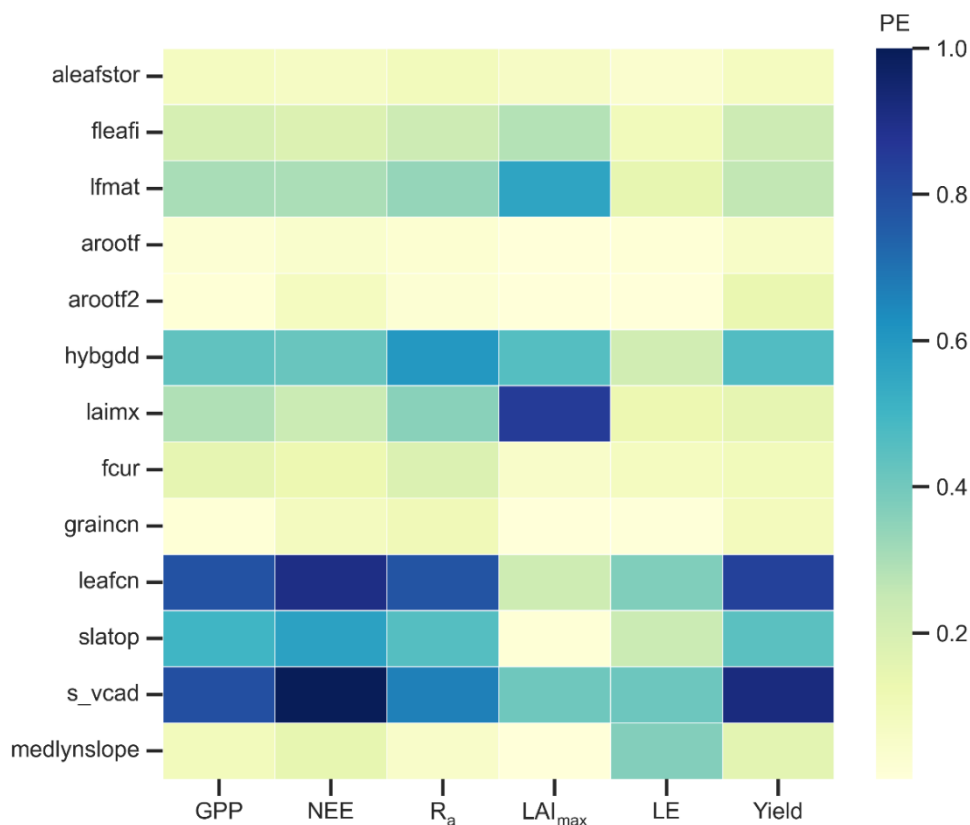


Figure 3.3 Parameter effect (PE) as a measure of sensitivity of selected output variables to the most influential model parameters. Output variables include gross primary production (GPP), net ecosystem exchange (NEE), autotrophic respiration ( $R_a$ ), maximum leaf area index ( $LAI_{max}$ ), latent heat flux (LE) and yield. Parameters are: Post-harvest leaf allocation coefficient to storage (aleafstor), initial leaf allocation coefficient (fleafi), GDD to canopy maturity (lformat), root allocation coefficients at the start of fruit development (arootf) and until harvest (arootf2), GDD needed until harvest (hybgdd), maximum LAI (laimx), fraction of allocation that goes to currently displayed growth (fcur), C:N ratios of fruits (graincn) and leaves (leafcn), specific leaf area at top of canopy (slatop), slope of the relationship between leaf N per unit area and the maximum rate of carboxylation at 25 °C ( $s\_vcad$ ), and the medlyn slope of the conductance–photosynthesis relationship (medlynslope). For more details on the parameters, see Appendix V.

### 3.3.2 Modelling results

In the following, we present the modelling results according to the initial parameterization and the updated parameter values from the sensitivity analysis. Daily simulations or yearly sums are compared to observed biomass, yield, and LAI data as well as ecosystem fluxes retrieved from the EC measurements and the SM measurements aggregated to daily mean values.

#### 3.3.2.1 Biomass growth and yield

The patterns in seasonal biomass allocation simulated by CLM5-FruitTree show good agreement with the monthly observations from 2010 (Figure 3.4a). The beginning and end of the growing season are well captured. After bud break at the beginning of March, biomass is allocated to the vegetative organs of leaves, fine roots, and woody organs, and growth is supported by C and N reserves until the start of fruit growth in early May (50 days according to the *ndays\_stor* parameter). In the following months, fruit biomass grows rapidly until harvest takes place in mid-October, following the typical sigmoidal growth curve that is well captured by the new phenology and CN allocation. Simulated leaf biomass peaks in mid-June and remains constant thereafter, with leaf senescence starting later October when temperatures drop below 4 °C. Pruning is performed when the tree enters dormancy by removing 85% of the stem biomass assimilated over the season according to the observed pruning amounts in the studied apple orchard [Zanotelli *et al.*, 2015; Zanotelli *et al.*, 2013]. From 2010 to 2012, the modelled percentage of biomass allocation to plant organs was generally in agreement with the observations [Zanotelli *et al.*, 2015], with differences ranging between 1 and 5% for fruits, leaves, aboveground wood, and roots (Figure 3.4b). Penzel *et al.* [2020] stated that different studies reported biomass allocation to fruits ranging from 50 to 85% depending on apple cultivar, suggesting considerable variability in allocation coefficients. This emphasizes the benefit of a cultivar specific calibration in order to obtain realistic modelling results. On the other hand, it suggests that a more general parameterization, that reflects an average apple tree, may be necessary to apply CLM5-FruitTree at larger scales and across multiple cultivars.

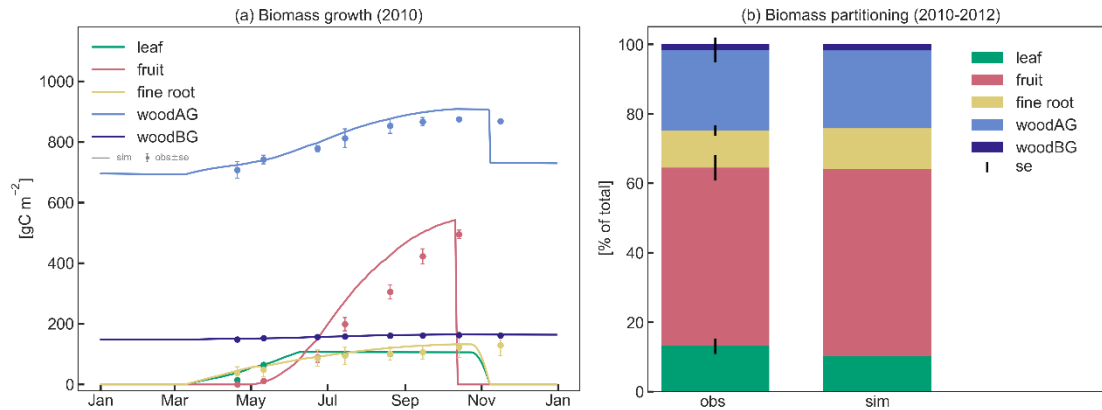


Figure 3.4 (a) Observed and simulated growth of leaves, fruits, fine roots, aboveground (live and dead stem), and belowground biomass (live and dead coarse roots) during 2010. (b) Observed and simulated biomass components between 2010 and 2012 as percentage of total biomass.

The timing for initial leaf development in spring and leaf senescence in late autumn are sufficiently well captured by the implemented bud break prediction algorithm and the simple temperature threshold for leaf abscission, respectively (Figure 3.5). Observed maximum LAI varied between 2.8 and 3.3  $\text{m}^2 \text{m}^{-2}$  and occurred during the first half of July. The simulations reached similar values in 2010 and 2012, matching the observations, while the simulated LAI in 2011 underestimated the measurements due to a smaller C transfer from storage and lower solar radiation early in the growing season. The discrepancy between the low simulated LAI and the high observed LAI in 2011 could have been further exacerbated by a lighter pruning performed in the previous winter compared to other years [Zanotelli *et al.*, 2013]. Such practice is sometimes performed in an attempt to counteract the strong alternate bearing behaviour of the Fuji variety, which causes a substantial drop in yield following a high yielding year [Atay *et al.*, 2013; Belleggia *et al.*, 2009; Pasa *et al.*, 2021]. As a consequence of the light pruning, a larger number of vegetative and flower buds remained on the tree, leading to more growth and possibly contributing to the larger discrepancy between relatively high observed LAI and relatively low simulated LAI. The adjusted pruning is however based on a somewhat subjective assessment of the farmer and information about the exact amount is hardly available. Thus, CLM5-FruitTree currently adopts a simplified pruning practice based on the removal of a fixed portion of the seasonal stem growth which manages tree size and total woody biomass without affecting LAI.

Measured LAI showed a slow decline soon after maximum LAI was reached, while simulated values in contrast are assumed to remain constant until leaf senescence is initiated. The observed early decline may be an artefact of the sampling strategy used to



determine LAI that extrapolated individual leaf area measurements to the whole tree, assuming a constant leaf distribution within the tree [Zanotelli *et al.*, 2013]. Another reason could be some premature leaf fall in the summer at the expense of the inner shadowed leaves, as observed during field sampling. Other studies suggest that the LAI of fruit trees generally stays constant until a rapid decline with the start of senescence [Lakso *et al.*, 1999; Pallas *et al.*, 2016], supporting the simulated LAI dynamic.

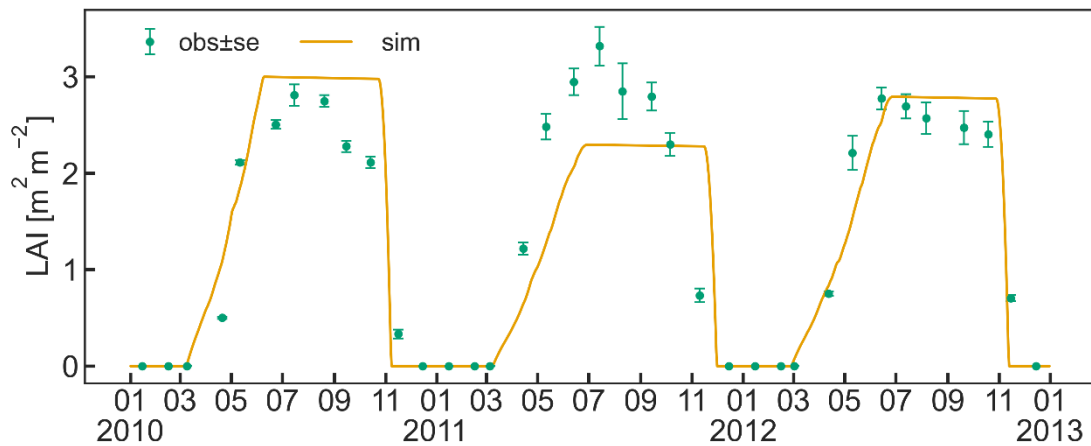


Figure 3.5 Simulated daily leaf area index (LAI) between 2010 and 2012 together with observations ( $\pm$ standard error) of LAI that were made once a month for the same period. Ticks on the x-axis refer to the beginning of the month.

Simulated yield averaged  $70 \text{ t ha}^{-1}$  between 2010 and 2015 and was within 2.3% of the observed average yield. While simulated yield varied between  $61$  and  $76 \text{ t ha}^{-1}$ , the observations showed a greater inter-annual variability (IAV), as exemplified in the case of the years 2012 (low yield of  $51 \text{ t ha}^{-1}$ ) and 2015 (high yield of  $101 \text{ t ha}^{-1}$ ) (Figure 3.6). Low IAV of yield has also been observed in previous crop simulations with CLM5 for winter wheat [Boas *et al.*, 2021] suggesting that certain drivers of IAV such as extreme environmental conditions (e.g., frost, heat, and hail) or plant pests and diseases and the resulting plant physiological responses (e.g., stress-induced leaf shedding or failure to flower) [Charrier *et al.*, 2021] are missing or not represented with sufficient detail in CLM5. In the case of apple trees, yield is also tightly linked to the number of flowers and early fruit growth, which in turn depend on a complex interaction of the environmental conditions during winter dormancy and the start of the new growing season [Chmielewski *et al.*, 2012; Corelli-Grappadelli and Lakso, 2002]. Additionally, C reserves accumulated in the previous year [Greer *et al.*, 2002], and crop load management play an important role in determining the final harvest [Penzel *et al.*, 2020]. The latter includes pruning or fruit thinning to ensure optimal fruit growth and to reduce the effect of alternate bearing.

The low observed yield in 2012 may be a result of such behaviour. This phenomenon and the processes involved are not universal, so that different fruit trees may be bearing regularly, irregularly, or biannually [Hoblyn *et al.*, 1937; Monselise and Goldschmidt, 1982]. As such, alternate bearing and its treatment through pruning or fruit thinning cannot easily be generalized and are thus not currently implemented in CLM5-FruitTree, which could have further reduced simulated IAV. Storage growth is considered in CLM5-FruitTree and exhibited an impact on the final yield of the following season, as shown by the sensitivity analysis of the *aleafstor* and *fcur* parameters (Figure 3.3). However, its effect on fruit growth in CLM5-FruitTree is indirect since it supports leaf development in the early growth stage but does not directly contribute to fruit growth. Identifying the driving forces of reserve deposition and mobilization and their quantification remains an unsolved issue, and there is yet no consistent formulation of this process in tree modelling [Allen *et al.*, 2005; Le Roux *et al.*, 2001]. Predicting final yield in fruit orchards is further complicated by the fact that harvest is usually based on certain fruit quality traits such as firmness or soluble solids and can occur successively as fruits may not mature at the same time [Corelli-Grappadelli and Lakso, 2002; Musacchi and Serra, 2018]. Within this context, the proposed simplifications of the C reserve dynamics and fruit harvest are likely contributing to the difference in observed and simulated yields. Considering the many specific challenges in modelling this apple cultivar, we believe that the yield predictions are satisfactory enough in the context of the sub-model development.



Figure 3.6 Annual yields from 2010 to 2015 and their mean in tons of fresh weight per hectare. For the conversion of simulated fruit biomass in gram carbon per square metre to tons per hectare, fruit C content was assumed 42% of total dry weight, harvest efficiency was assumed 95%, and fruit water content 83% according to Zanotelli *et al.* [2013].

### 3.3.2.2 Ecosystem fluxes and soil moisture variation

#### Carbon fluxes

As shown in Figure 3.7, CLM5-FruitTree was able to capture the overall patterns of GPP, NEE, and  $R_{eco}$ , particularly during the transition between dormancy periods and growing seasons (April to November). Simulated C fluxes are highly correlated with observations ( $r \geq 0.84$ ) while the RMSE ranges between 1.12 and 1.53  $\text{gC m}^{-2} \text{d}^{-1}$ . Observed and simulated peak C fixation occurred in mid-June (Figure 3.7a), corresponding to the maximum (negative) NEE (Figure 3.7c) and maximum LAI (Figure 3.5). Simulated NEE becomes negative (net carbon sink) around April and returns to positive (net carbon source) around November, in agreement with the observed dynamic (Figure 3.7c). Observed yearly sums of GPP (NEE) were 1.60 (−0.49), 1.43 (−0.48), and 1.65 (−0.76)  $\text{kgC m}^{-2} \text{yr}^{-1}$  for 2013, 2014, and 2015, respectively. Simulated yearly sums of GPP (NEE) were 1.58 (−0.53), 1.56 (−0.51), and 1.53 (−0.57)  $\text{kgC m}^{-2} \text{yr}^{-1}$  for the same years, showing a negligible positive bias of on average 0.17% for GPP (Figure 3.7b) and a small underestimation (less negative) of on average 3.8% for NEE (Figure 3.7d). Simulated and observed  $R_{eco}$  (Figure 3.7e) generally increased until July because of the increase in air temperature and respiratory costs of the developing canopy, and declined thereafter as air temperature started to drop. Simulations of  $R_{eco}$  tend to slightly underestimate observations between April and late August and to overestimate observations during winter, although discrepancies are relatively small. Observed yearly sums of  $R_{eco}$  were 1.13 (2013), 0.98 (2014), and 0.94 (2015)  $\text{kgC m}^{-2} \text{yr}^{-1}$ , while simulated values were 1.08, 1.08, and 0.99  $\text{kgC m}^{-2} \text{yr}^{-1}$ , respectively. CLM5-FruitTree overestimated yearly  $R_{eco}$  by on average 3.3%, explaining most of the difference in observed and simulated NEE in 2013, while differences in 2014 and 2015 are due to a combination of small biases in both GPP and  $R_{eco}$ . Measured  $R_{eco}$  showed irregular fluctuations in the early part of the growing season 2013 and mid to late season 2014 and 2015 that are not reproduced well by the model. These fluctuations mostly correspond to the observed temperature dynamics (not shown) as a result of the applied gap filling that is based on an air (or soil) temperature- $R_{eco}$  relationship [Reichstein *et al.*, 2005]. Such discrepancies between observed and simulated dynamics could be further explained by the occurrence of field management practices such as mowing of the grassed alleys or soil tillage under the tree rows, which are currently not represented in CLM5-FruitTree. Such practices could have led to a temporary rise in soil respiration ( $R_s$ ) due to increased heterotrophic respiration

( $R_h$ ) as discussed in *Zanotelli et al.* [2013]. Indeed, soil tillage experiments performed in an apple orchard located in a Loess plateau in Shaanxi Province in China were found to increase  $R_s$  14–57% depending on the tillage method [*Hou et al.*, 2021].

*Zanotelli et al.* [2013] measured a total  $R_s$  of  $801 \pm 95$  gC m<sup>-2</sup> in 2010, contributing around 90% to  $R_{eco}$ , based on soil chamber measurements within the orchard (total soil respiration). The comparison to parallel measurements in a trenched plot produced a high ratio  $R_h/R_s$  of 0.77 for the apple orchard. In contrast, simulated  $R_s$  was 510 gC m<sup>-2</sup>, contributing merely 45% to  $R_{eco}$  for the same year with a ratio  $R_h/R_s$  of 0.87. Simulated  $R_{eco}$  was instead dominated by autotrophic respiration ( $R_a$ ) due to high C costs for maintenance, mainly of leaf biomass (data not shown). Other studies found that  $R_s$  contributed 56–67% to  $R_{eco}$  in irrigated citrus orchards of different ages that share common management practices (i.e., use of heavy machinery, irrigation, fertilization, tree pruning, and mulching) as well as structural similarities (e.g. planting in tree rows) with the studied apple orchard. Both aspects have a strong influence on soil respiration components in orchards [*Martin-Gorriz et al.*, 2020]. In forest ecosystems, where the magnitude of ecosystem fluxes was found to be somewhat comparable to orchards,  $R_s$  contributed > 60% to  $R_{eco}$  [*Lasslop et al.*, 2012; *Zanotelli et al.*, 2013].

In addition to the missing representation of certain management practices, CLM5-FruitTree currently does not account for an active ground cover in the orchard, which has shown to enhance  $R_s$  in an Italian olive orchard through increased fine root and microbial biomass [*Turrini et al.*, 2017]. Furthermore, the simplified representation of microbial activity in CLM5, through fixed respiration fractions for litter and soil organic matter pools, may limit the ability of CLM5-FruitTree to accurately represent soil respiration processes. Not accounting for mycorrhizal respiration may fail to adequately represent  $R_{eco}$  of the orchard, as measurements suggested a substantial contribution of  $11 \pm 6\%$  to total  $R_s$  in an apple orchard [*Tomè et al.*, 2016]. Lastly, biases in simulated soil temperature, SM content, and fine root density could further contribute to explaining the above discussed differences, as these factors have a major effect on  $R_s$  in apple orchards [*Ceccon et al.*, 2011].

In contrast to the underestimation of  $R_s$  in the model, the simulated  $R_a$  of 693 gC m<sup>-2</sup> was almost twice the measured value of  $372 \pm 195$  gC m<sup>-2</sup>. In our simulations, maintenance respiration comprised the main part of  $R_a$ , with on average 78%. The calculation of

maintenance respiration in CLM5 (see Section 3.2.1) does not account for a lower or varying maintenance cost observed in mature apple orchard canopies compared to annual crops [Bepete and Lakso, 1996; Lakso et al., 1999]. It therefore seems likely that the tissue maintenance costs in the orchard are overestimated in CLM5-FruitTree, accounting for on average 45% of  $R_a$  (28% of  $R_{eco}$ ). This could also explain the lower simulated carbon use efficiency (NPP/GPP) of 0.59 compared to 0.71 found by Zanutelli et al. [2013]. Further work and more experimental data are needed to better understand the differences in modelled and observed respiration partitioning and to improve the performance of CLM5-FruitTree to adequately simulate the respiration components in fruit orchards.

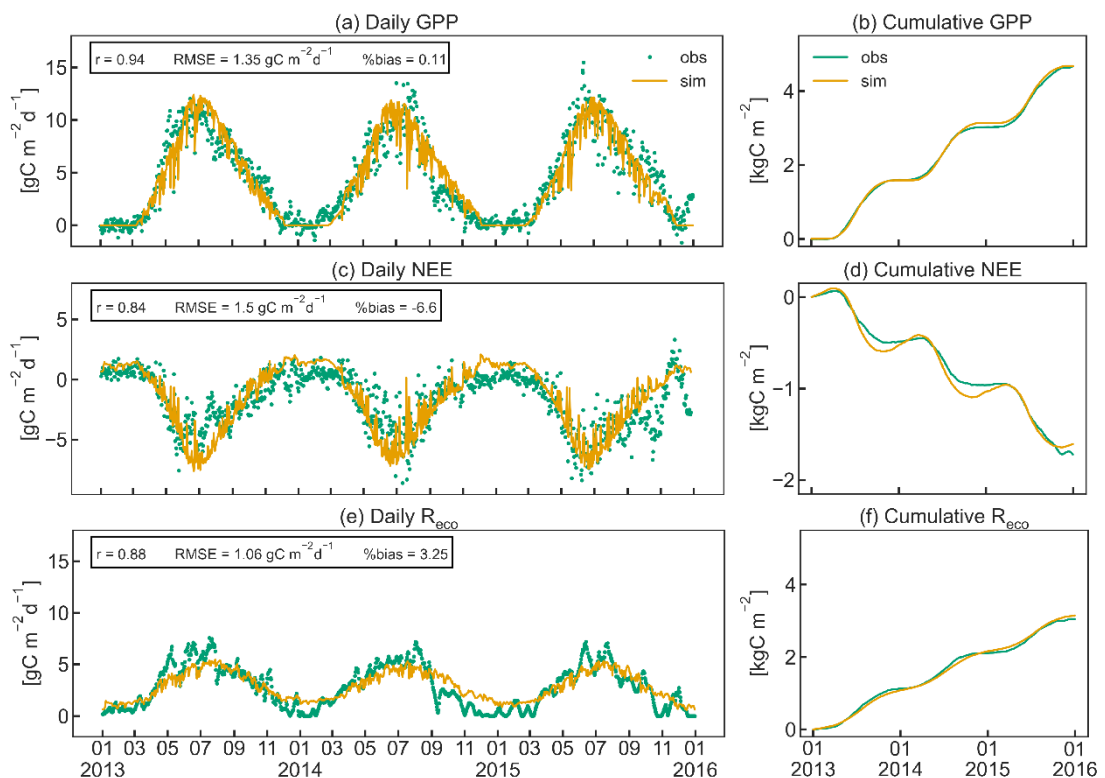


Figure 3.7 Daily instantaneous (a, c, e) and cumulative (b, d, f) observed and simulated fluxes of gross primary productivity (GPP), net ecosystem exchange (NEE), and ecosystem respiration ( $R_{eco}$ ) for the studied apple orchard between 2013 and 2015. Pearson's coefficient of correlation ( $r$ ), the root mean square error (RMSE) and the percent bias (%bias) are displayed as statistical indices.

### Energy and water fluxes

The simulated seasonal course of the energy balance components  $R_n$ ,  $G$ ,  $LE$ , and  $H$  agrees well with observed dynamics in the orchard (Figure 3.8). CLM5-FruitTree shows a high performance in reproducing  $R_n$  and  $LE$  with  $r \geq 0.97$  and RMSE of 15.98 and 17.85  $W m^{-2}$ , respectively (Figure 3.8a and c). Due to the lack of  $LW_{in}$  measurements, the CLM5 internal  $LW_{in}$  calculation based on a clear-sky parameterization after Idso [1981] was used initially. This resulted in a significant underestimation of 5% (511 MJ) for  $LW_{in}$  and

18% (471 MJ) for  $R_n$  compared to the observations in 2010. The  $R_n$  bias could be reduced by 14% for the observed time series when  $LW_{in}$  was calculated by considering cloud cover as described in Appendix IV. This stresses the necessity of accounting for cloud cover, ideally combined with locally calibrated parameters, for an accurate calculation of  $LW_{in}$ . The remaining small negative bias of 4.48% in  $R_n$  is due to negative simulated  $R_n$  during the winter months (Figure 3.8b), which may be a result of the higher reflectance of solar radiation from bare soil compared to a grass surface [Bryś *et al.*, 2019]. The model assumes a bare soil (except for stem area) during the dormancy period, as the grass-covered alleys in the orchard are not considered explicitly.

The simulated LE (Figure 3.8c) shows similar dynamics and variability to the observations following the increase and decrease in GPP (Figure 3.7a) and LAI (Figure 3.5). Similarly to LE, modelled ET shows a high correlation coefficient of 0.97 and a small RMSE of 0.62 mm d<sup>-1</sup> (Figure 3.8i). Simulated ET exceeds observed ET by 1.1 mm d<sup>-1</sup> on average during its peak in July, but the overall bias is almost negligible (Figure 3.8j). Total observed ET is 901 (2013), 858 (2014), and 883 (2015) mm, while the corresponding simulated values are 916, 877, and 925 mm, respectively. When examining the order of magnitudes of the ET components, canopy transpiration takes up around 85% of ET, followed by soil evaporation and canopy evaporation (data not shown). Typically, apple orchard ET represents a combined flux from the apple trees and the grassed alley system, which is not explicitly represented in CLM5-FruitTree since CLM5 currently does not consider inter-row grass coverage or intercropping. Ntshidi *et al.* [2021] found that the contribution of understory transpiration is high in young, non-bearing apple orchards but contributes less than 10% to whole-orchard ET in mature orchards with high canopy cover, which may explain the good model performance despite not considering the grass cover.

Simulated H and G are less consistent with the observations with r values of 0.54 and 0.64, respectively, and large percent bias (Figure 3.8e and g), which is partially due to the much smaller magnitudes of the two fluxes compared to  $R_n$  and LE. A possible reason for the lower amplitude of observed G (Figure 3.8h) compared to simulated values may be the dampening effect of the grass cover providing additional shading during summer and insolation during winter [Bryś *et al.*, 2019; Oorthuis *et al.*, 2021]. Observed H was rather constant throughout the year, with slightly higher values at the start and end of the growing season when the canopy was not yet fully developed or leaves were shedding.

CLM5-FruitTree simulated a clear rise of H until April, closely following the observations, but H thereafter declined steeply in May, with negative values in August 2013 and 2015. Negative H during August corresponds to maximum LE and the main simulated irrigation season (June to September) that added 357 (2013), 281 (2014), and 517 mm (2015) of water to the orchard (Figure 3.9a). In a study conducted with CLM4.5, intense irrigation was found to strongly influence the convective heat fluxes by increasing LE and decreasing H [Zeng *et al.*, 2017]. Although precise measurements of the irrigation amount in the orchard are not available for the studied period, the average yearly irrigation was estimated around 200 mm, with no irrigation in 2014 due to sufficient rainfall [Montagnani *et al.*, 2018]. The difference in irrigation amounts may in part explain why the described phenomenon is not observed in the measurements. Indeed, negative simulated H in the summer months occurred as a result of strong evaporative cooling of ground and vegetation temperature through energy absorption by LE following irrigation that caused simulated LE to exceed simulated  $R_n$ . This behaviour was not observed in the measurements where LE rarely exceeded  $R_n$  and was mostly due to an overestimation of simulated LE compared to the measurements. Persisting model weaknesses in the partitioning of the energy balance were pointed out by a recent study examining land surface processes over a tropical rainforest using CLM4.5 and CLM5, and were linked to missing detail in the representation of the canopy and an oversensitivity of vegetation temperature to incoming solar radiation, among others [Song *et al.*, 2020]. As a result, the authors observed an overestimation of LE and unrealistically high day-to-night changes in G, which was also observed in this study when examining the model output at an hourly time step (results not shown).

Energy partitioning in orchards is strongly influenced by the positioning and pruning of branches to optimize tree architecture for higher productivity, planting density, tree height, and LAI distribution [López-Olivari *et al.*, 2016]. Consequently, the contribution of H and LE can significantly differ in the discontinuous orchard canopy (grass-covered alleys between tree rows) compared to the closed canopies of annual crops [la Fuente-Sáiz *et al.*, 2017]. Currently CLM5 is still limited to the assumption of a closed canopy structure that is uniform in space, and hence biases are likely to arise from this model limitation. Future developments towards integrating multi-layer schemes for canopy processes and the explicit representation of the canopy to improve the related processes are desirable for a more realistic representation of the orchard canopy structure.

### **Soil moisture variation**

Simulated mean SM at 5 cm depth was within 1.6% vol of the observed value during the three observed growing seasons, despite the higher simulated irrigation amount (Figure 3.9b). Simulated daily values show a greater variability than the measured data in response to precipitation and to frequent irrigation (Figure 3.9a–b). In contrast, observed SM in the deeper soils (30–60 cm), was 3–11% vol higher during the growing season compared to simulated values (Figure 3.9c–d). Considering the total investigated soil depth, simulations exhibit a larger variability in SM throughout the year, with a general overestimation in winter and underestimation during the growing season (especially in the deeper soils). However, the collected SM data were limited to a single soil profile that may not adequately reflect the average SM of the apple orchard, which should be considered when comparing measurements and simulations. Even though the measurements are incomplete, the constant high observed SM in the deeper soils suggests an ample supply of water due to capillary rise from the shallow groundwater table that typically ranges between 1.2 and 1.85 m in the area [Montagnani *et al.*, 2018]. This process replenishes the water removed by ET processes and may explain the reduced need for irrigation compared to the simulations. Despite the shallow simulated ground water table (generally 1.2 m depth), groundwater could not be used for root water uptake in the simulation as the rooting depth of the orchard was restricted to 0.8 m according to local measurements, and capillary rise is currently not implemented in CLM5.



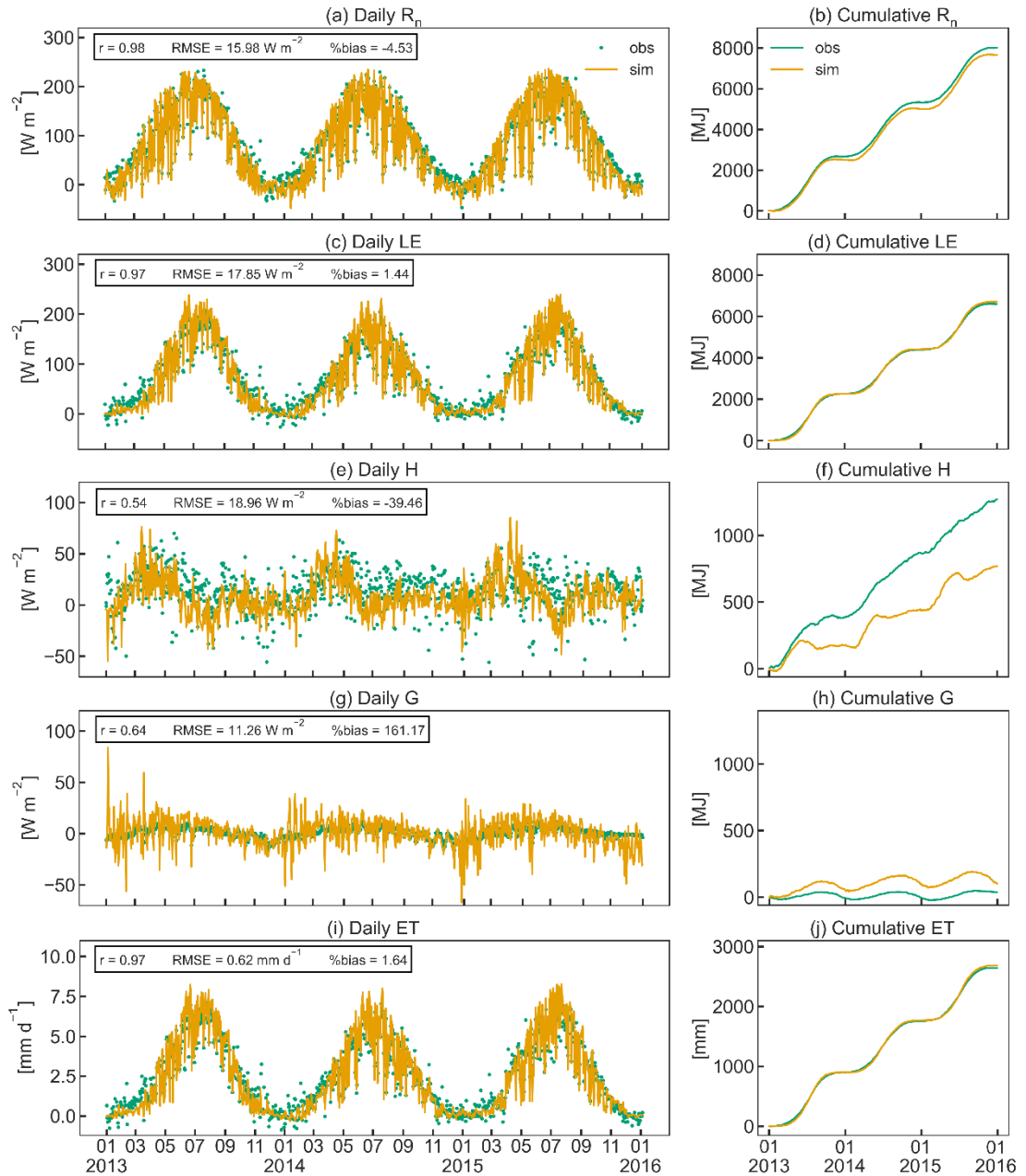


Figure 3.8 Daily and cumulative observed and simulated fluxes of net radiation ( $R_n$ ), ground heat ( $G$ ), latent heat ( $H$ ), sensible heat ( $LE$ ) and evapotranspiration ( $ET$ ) for the studied apple orchard between 2013 and 2016

2015. The coefficient of determination ( $r$ ), the root mean square error (RMSE) and the percent bias (%bias) are displayed as statistical indices.

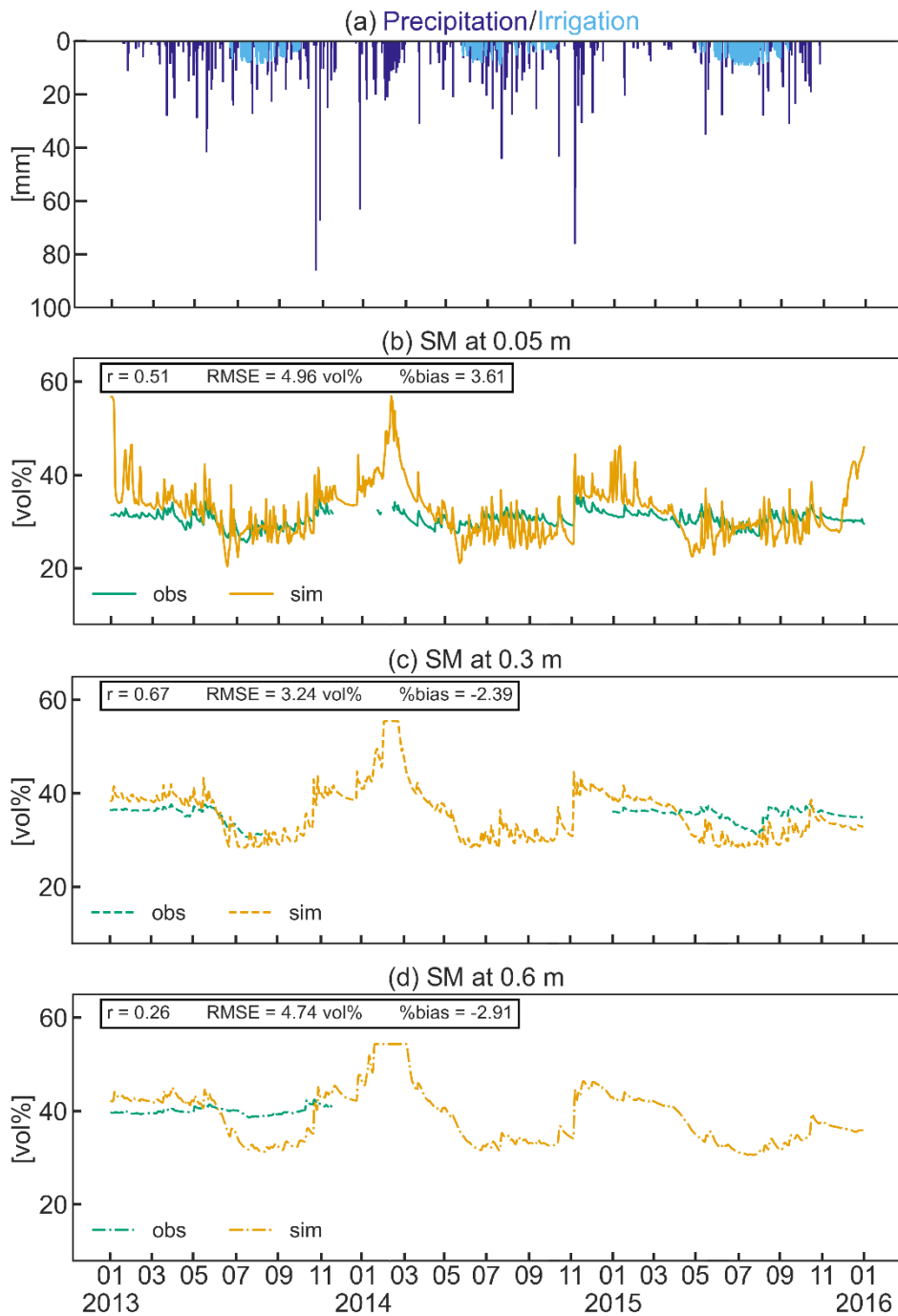


Figure 3.9 Precipitation and simulated irrigation (a), and observed and simulated soil moisture (SM) at 0.05 m (b), 0.3 m (c), and 0.6 m (d) depth from 2013-2015.

### 3.4 Conclusions

The novel CLM5-FruitTree was developed to model perennial deciduous fruit orchards and thus extended the representation of agricultural systems in CLM5. The development included a new phenology subroutine to account for the perennial nature, prolonged growing season, and distinct phenological development of fruit trees compared to annual crops. Furthermore, C reserve dynamics of perennial deciduous trees were considered by adapting the CN allocation and typical management practices associated with fruit orchards were represented, such as transplanting of seedlings and winter pruning. To evaluate the development, a new apple PFT was parameterized, and the model was set up and tested using extensive site data of a mature apple orchard in northern Italy.

One-by-one parameter sensitivity analysis revealed that photosynthetic parameters and parameters associated with canopy conductance have the highest influence on GPP, NEE, LE, and yield, while phenological parameters were more influential in biomass partitioning to the different plant organs. Due to the high number of model parameters and parameter covariation, future studies could propose a more comprehensive sensitivity analysis with a training data set consisting of multiple sites, which would give more insight into model sensitivity and could further improve the parameterization.

CLM5-FruitTree was able to capture the seasonal biomass development as well as the average relative partitioning of the total biomass into the different plant organs. The inclusion of C reserves next to photosynthetic growth was imperative to enable regrowth at the end of a dormancy period and influenced LAI development, total seasonal biomass, and yield. Average simulated yield was within 2.3% of the observation even though CLM5-FruitTree showed a lower IAV likely due to the simplification of C reserve dynamics, specific management practices, and the alternate bearing behaviour exhibited by the Fuji apple cultivar.

The new phenology and CN allocation algorithms well represented the seasonal course of carbon, water, and energy fluxes of the orchard. The magnitude of ecosystem fluxes was particularly well captured for GPP,  $R_n$ , LE, and ET, with correlation coefficients  $> 0.94$  and percent bias  $< \pm 5\%$ . The model exhibited small biases in NEE and  $R_{eco}$  that were most likely caused by the overestimation of  $R_a$ , especially leaf maintenance respiration, and an underestimation of  $R_s$ . Possible reasons for the smaller simulated contribution of  $R_s$  to  $R_{eco}$  could be the missing representation of the grass-covered alleys, differences in

simulated and actual soil temperature or organic matter content, and oversimplification of microbial respiration processes. Additionally, large negative biases in simulated H were found over most of the main irrigation season during summer as the model simulated a strong evaporative cooling of the surface temperature.

Further model developments should consider the improvement of canopy processes related to energy partitioning and the inclusion of an active ground cover in the orchard representation to improve the yearly energy budget calculations and possibly soil respiration. An explicit representation of the microbial community and a more flexible calculation of  $R_a$ , i.e. considering tissue age, should also be the focus of future model improvements. While the particular alternate bearing of the Fuji variety posed a challenge in this specific study, the pruning routine that is currently implemented may be sufficient for most other apple cultivars and fruit tree species for which this behaviour is less pronounced or not exhibited. However, future developments could be envisioned once the model is further tested and applied. In addition, management practices such as mowing or soil tillage could further enhance the model capability of capturing the dynamics and fate of assimilated C. Fruit thinning is another common practice in orchards, but its implementation would be more challenging, as the current model structure does not represent individual fruits. This process could however be implicitly accounted for through parameterization of the C allocation to fruits. Finally, the application of the newly developed sub-model to different geographical regions and other types of fruit trees or apple cultivars is needed to further validate the model and give more insight into the transferability of the development to different types of orchards.

Overall, our results demonstrate the ability of the newly developed CLM5-FruitTree sub-model to represent the seasonal dynamics and magnitudes of growth and ecosystem fluxes in a deciduous fruit orchard. As such, this development constitutes an important contribution to a more comprehensive representation of the agricultural land surface in CLM5 by adding a perennial, woody crop to the existing annual crop types. This will allow for a more realistic evaluation of land use and climate change effects, or water availability at regional scale such as the Mediterranean or parts of China and the US, where perennial agriculture such as fruit orchards covers large parts of the agricultural landscape.

# 4 Land surface modelling as a tool to explore sustainable irrigation practices in Mediterranean fruit orchards

This chapter is based on the following manuscript:

**Dombrowski, O.**, Brogi, C., Hendricks Franssen, H. J., Bogena, H., Pinaras, V., Panagopoulos, A., Chatzi, A., Babakos, K. & Swenson, S. (2023). Land surface modelling as a tool to explore sustainable irrigation practices in Mediterranean fruit orchards. (submitted to Water Resources Research)

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## Abstract

Irrigation strongly influences land-atmosphere processes from regional to global scale. Therefore, an accurate representation of irrigation is crucial to understand these interactions and address water resources issues. While irrigation schemes are increasingly integrated into land surface models, their evaluation and further development remains challenging due to data limitations, e.g. irrigation amounts and timing, and soil moisture (SM). This study assessed the representation of irrigation and its effect on crop yield in the Community Land Model version 5 (CLM5) through implementation of an irrigation data stream that allows to directly use observed irrigation data. Simulations were conducted at the point scale for two instrumented apple orchards using the CLM5 irrigation routine as well as the implemented data stream. Furthermore, irrigation requirements and the effect of deficit irrigation on crop yield and crop water use efficiency (CWUE) at the regional scale were simulated and discussed. The irrigation data stream performed better in representing observed SM dynamics compared to the standard irrigation routine that could be further improved by implementing more flexible irrigation schedules and irrigation efficiency. At the regional scale, simulated irrigation and yield showed a high sensitivity to climatic changes caused by the topographic gradient. While a 25% reduction in irrigation had negligible negative effect on simulated yield and CWUE, a reduction of 50% notably reduced both variables. These effects varied with climatic conditions, soil properties and timing of irrigation. These results showcase how CLM5 could be utilized for irrigation and water resources management.

## 4.1 Introduction

Irrigation plays a vital role in sustaining global food production by providing a reliable water supply to agricultural systems, especially in semi-arid or arid regions [McLaughlin and Kinzelbach, 2015]. With a growing global population and increasing food demands, irrigation contributes significantly to ensuring food security by enabling higher crop yields and reducing the vulnerability of agricultural systems to climate change [McDermid *et al.*, 2023; Mueller *et al.*, 2012]. On the other hand, poor management of irrigation water has led to the depletion of groundwater resources [Dangar *et al.*, 2021; Scanlon *et al.*, 2012; Wada *et al.*, 2010] and water use conflicts in many regions [Cai *et al.*, 2003; Eshete *et al.*, 2020; Gurung *et al.*, 2006]. Apart from quantitative and qualitative effects on water resources [García-Garizábal *et al.*, 2012; Zhang *et al.*, 2022], irrigation substantially impacts biogeophysical and biogeochemical processes at the land surface through alteration of the hydrological cycle or energy budget. This has subsequent effects on climate [DeAngelis *et al.*, 2010; Erb *et al.*, 2017; Ferguson and Maxwell, 2012; Gordon *et al.*, 2005; Sacks *et al.*, 2009]. The multidimensional role of irrigation calls for increased efforts in effective irrigation management and irrigation impact studies using large-scale approaches. This is crucial not only to meet food demands and mitigate future increases in climate change induced water stress, but also to understand its interactions and feedback mechanisms within the Earth system [Elliott *et al.*, 2014; McDermid *et al.*, 2023].

Modelling can be a powerful tool to simulate complex interactions in agricultural systems, evaluate different irrigation and climate scenarios, and provide decision support for water resources management [Blyth *et al.*, 2021; Pongratz *et al.*, 2018]. This necessitates comprehensive modelling frameworks that combine field-scale representations of crop growth and irrigation with a more holistic assessment of the impacts of irrigated agriculture on water resources and climate at larger scale [Peng *et al.*, 2020]. Process-based crop models include a range of crop parameterizations that provide a unique way to study crop growth processes in response to irrigation practices by using physical and biological principles. However, their main purpose is to simulate yield at the field scale, often over a single growing season, while lacking the interface with the land surface, soil, and climate [Cheng *et al.*, 2020]. Land surface models (LSMs), on the other hand, provide a more holistic representation of the land-atmosphere interactions to capture the feedback mechanisms between irrigation, vegetation,

hydrological processes, and climatic conditions beyond the field scale [Blyth *et al.*, 2021]. Conversely, they often lack more detailed physiological and genetic representations of crops and irrigation management [Lombardozzi *et al.*, 2020; Peng *et al.*, 2018]. This limits the ability of LSMs to reliably simulate yield and irrigation water withdrawals leading to poor model performance and biases in related processes such as carbon, energy, and water fluxes over intensively irrigated regions [Leng *et al.*, 2015; Lombardozzi *et al.*, 2020; Ozdogan *et al.*, 2010; Zhang *et al.*, 2020].

In recognition of the important role of human land management, efforts to advance the representation of crops and irrigation in LSMs are ongoing [Pokhrel *et al.*, 2016]. Various land surface models such as ORCHIDEE, the Community Land Model (CLM), and Noah-MP have since added crop modules [Levis *et al.*, 2012; Liu *et al.*, 2016; Smith *et al.*, 2010]. New crop representations have been developed to improve crop growth and management processes [Boas *et al.*, 2021; Peng *et al.*, 2018] or to add new crop types [Dombrowski *et al.*, 2022; Fader *et al.*, 2015; Fan *et al.*, 2015]. Rather simple irrigation schemes are generally incorporated based on soil moisture (SM) thresholds [de Vrese *et al.*, 2016; Ozdogan *et al.*, 2010; Sacks *et al.*, 2009], while more recent developments include the integration of irrigation techniques [Leng *et al.*, 2017; Yao *et al.*, 2022], irrigation water withdrawal from different sources [Leng *et al.*, 2017; Xia *et al.*, 2022], and water availability limitation [Yin *et al.*, 2020]. These studies, however, were performed at river basin, county, or global level with coarse spatial resolutions between 10 and 100 km. Simulated irrigation was validated against rather uncertain statistics like total yearly irrigation water withdrawals, without considering specific irrigation practices. Crop and irrigation data at higher spatial (< 5 km) and temporal (e.g. daily or sub-seasonal) resolution is needed to evaluate the representation of local irrigation schedules in LSMs and support irrigation management decisions. However, data to reliably constrain and further develop implemented irrigation schemes is often lacking, e.g. irrigation amount and timing along with continuous SM observations [Lawston *et al.*, 2017]. Lawston *et al.* [2017] first evaluated the sprinkler irrigation scheme of the NASA Land Information System LSM with point and gridded SM observations at 1 km resolution. While the model could not capture the field-scale heterogeneity and overestimated irrigation amounts, it captured well the seasonal variability and regional average SM dynamics. The authors did however use a prescribed crop phenology (green vegetation fraction) and did not examine the effect of irrigation on crop yield. A recent study examined the effect of

different irrigation setups on maize yield and two water use efficiency definitions using the dynamic crop and irrigation scheme of the Noah-MP LSM [Huang *et al.*, 2022]. They found that modelled crop yield was sensitive to irrigation quantity and timing (in which crop growth stage irrigation was applied) and based on these results recommended an optimal SM threshold to trigger irrigation. While the authors lacked data to accurately assess the irrigation amount and crop yield, their work presents a first use of a LSM to study the effects of deficit irrigation on crop growth, yield and water use efficiency.

The work presented here builds upon previous studies to continue the evaluation and improvement of irrigation representations in LSMs combining local irrigation, SM, and yield observations. In particular, this study applies CLM version 5, with a recent extension to represent deciduous fruit trees, to model irrigation and crop growth in a Mediterranean catchment. Specifically, we aim to: (1) evaluate the existing irrigation scheme of CLM5 and enhance its flexibility to account for local irrigation management practices; (2) assess whether the model can reproduce SM dynamics and crop growth in irrigated apple orchards using the enhanced model capability; (3) examine the potential to improve regional irrigation management by modelling the effect of different irrigation scenarios on crop yield and water use efficiency at the catchment scale.

## 4.2 Materials and Methods

### 4.2.1 Study area

Located in central Greece, the Pinios Hydrologic Observatory (PHO) covers an area of approximately 45 km<sup>2</sup> (Figure 4.1). The PHO was established in 2015 to study the Pinios catchment hydrological processes and, ultimately, to support local authorities in the sustainable management of water resources [Pisinaras *et al.*, 2018]. It is characterized by a Mediterranean climate with an annual precipitation of 500 to 1200 mm, and highest precipitation amounts in the winter months, annual potential evapotranspiration of approximately 1100 mm, and annual average air temperature of 15 °C [Bogena *et al.*, 2018]. The area displays a range of altitudes from 1500 m in the northern part down to less than 200 m in the plain. The mountainous part of the catchment features steep slopes and is covered by forests, mixed with shrubs and grassland, while the southern plain is primarily characterized by agriculture and small villages. In the plain, sandy loam soils



dominate while sandy clay loam and loamy soils also occur [Pisinaras *et al.*, 2018]. The PHO is located in one of the most productive agricultural areas in Greece owing, among other factors, to widespread irrigation practices that account for over 85% of the local freshwater consumption [Panagopoulos *et al.*, 2018]. The main cultivation are apple and cherry orchards (i.e., ~78% of agricultural area) that are irrigated between May and October. There are a few other rainfed fruit and nut tree orchards in the area with < 5% coverage. Annual crops including corn, cereal (mainly winter wheat), and potato are grown on the remaining agricultural land. They are partially irrigated, depending on precipitation occurrence, but cover a negligible part of the total irrigated area. Irrigation in the orchards is typically applied through micro sprinklers and the demand is almost entirely met by abstraction from the alluvial groundwater system through water wells, most of which are privately owned. Overexploitation of groundwater in the area due to poor irrigation management practices, amongst others, has previously been reported by Panagopoulos *et al.* [2018] and Pisinaras *et al.* [2023] resulting in the decline of groundwater levels.

Within the PHO, irrigation management in two irrigated apple orchards, hereafter referred to as S09 and S10, was studied (Figure 4.1). Both orchards have a size of around 1.2 ha, with a mild southern slope of < 5%. The soil texture is sandy loam and sandy clay loam with a high gravel content (13–29%) (Table 4.1) and many larger cobbles (> 64 mm according to Wentworth [1922]), especially below 30–50 cm depth. Trees are planted in rows, oriented North-South with 3.3 m distance between rows and an in-line distance of 1.5 m (approximately 2020 trees ha<sup>-1</sup>). The trees in S09 and S10 were planted in 2013 and 2015 respectively, with a mixture of 3 to 5 different varieties. Trees are pruned to a height of 3.5 m throughout the winter season and residues are mulched back into the soil. Bud burst typically occurs in the second half of March while fruit development starts with the end of flowering in mid to late April. Harvest dates range from late August to mid-November depending on the harvested variety. Major leaf fall starts in late October and continues until mid-November, sometimes until early December. Trees are irrigated with a micro sprinkler system with a maximum flow rate of 60 L hour<sup>-1</sup> that is installed below the canopy, halfway between the tree stems of the same row. The irrigation season typically starts in May and continues until October. Orchards are fertilized with 80 kgN ha<sup>-1</sup> at the end of flowering in April. Pest and fungicide treatment is applied prior to flowering and after flowering until late June. The grass in the alleys is generally mowed

once a month starting in March or April and mowing material is left on the ground. During periods of intense heat, the actively growing grass cover provides a cooling effect to protect the apples from heat damage.

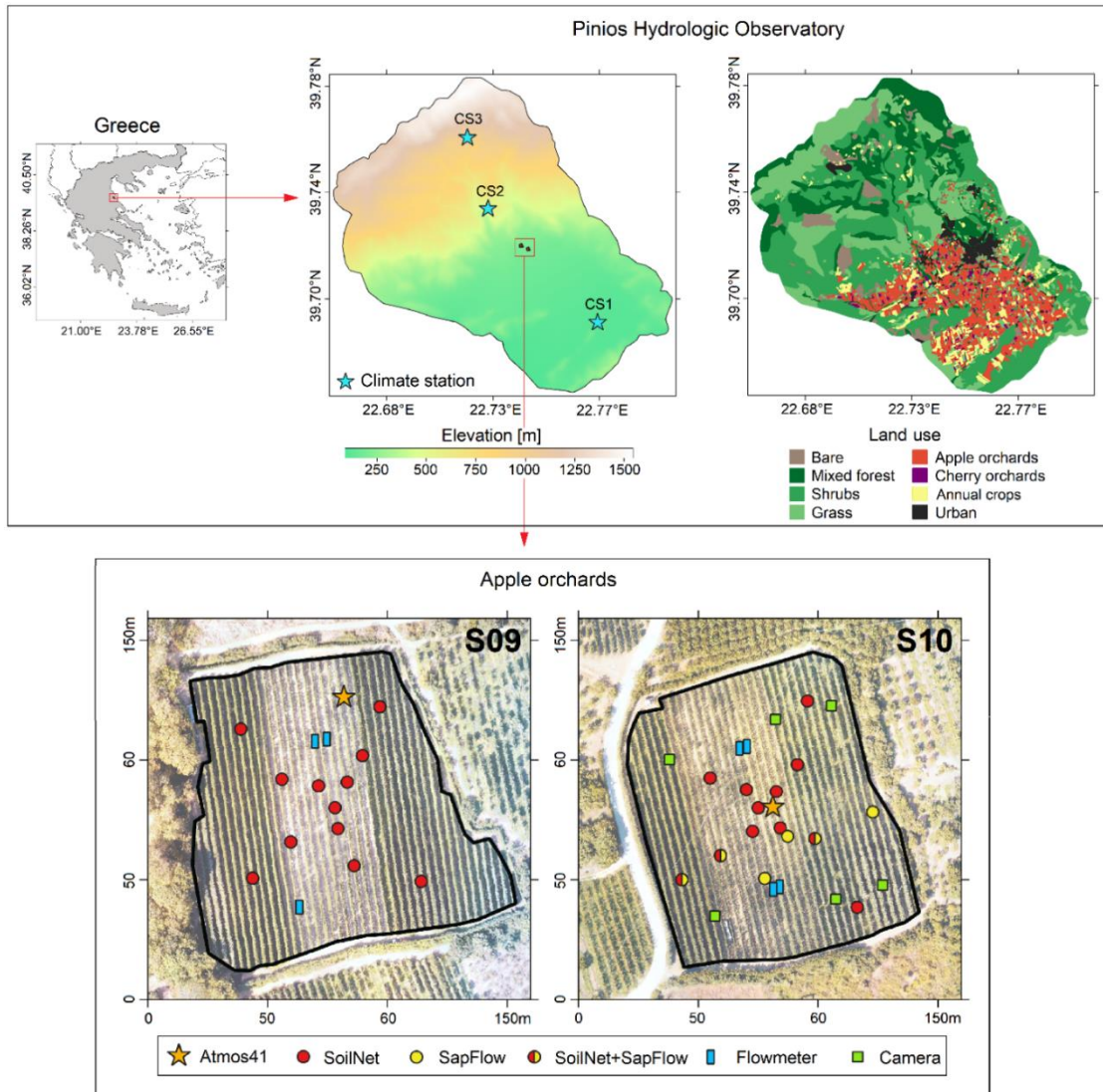


Figure 4.1 Top left: Map overview of Greece and of the study area location. Top right: Elevation and land use of Pinios Hydrologic Observatory with the locations of climate stations. Bottom: Apple orchards S09 and S10 with instrumentation.

Table 4.1 Main characteristics of the two apple orchards (S09 and S10).

| Orchard ID | Altitude (m a.s.l.) | Size (ha) | Apple varieties | Soil depth (cm) | Sand content (%) | Clay content (%) | Soil                       | Gravel content (%) |
|------------|---------------------|-----------|-----------------|-----------------|------------------|------------------|----------------------------|--------------------|
|            |                     |           |                 |                 |                  |                  | organic carbon content (%) |                    |
| S09        | 200                 | 1.24      | 3               | 0–30            | 64.5             | 17.8             | 1.5                        | 23.3               |
|            |                     |           |                 | 30–60           | 63.0             | 21.9             | 1.2                        | 20.6               |
|            |                     |           |                 | 60–90           | 59.9             | 24.6             | 0.7                        | 13.7               |
| S10        | 190                 | 1.13      | 5               | 0–30            | 64.3             | 12.5             | 1.44                       | 28.2               |
|            |                     |           |                 | 30–60           | 65.8             | 12.7             | 0.86                       | 28.7               |
|            |                     |           |                 | 60–90           | 65.4             | 13.7             | 0.66                       | 28.7               |

### 4.2.2 Data sources

The meteorological data that are necessary to drive CLM5 including precipitation, air temperature, atmospheric pressure, wind speed, relative humidity, and incoming solar radiation, were acquired from three meteorological stations located at different altitudes within the PHO (Figure 4.1) as well as two stations located in the orchards S09 and S10. For the agricultural plain, detailed soil texture and organic matter information was collected during an extensive soil sampling campaign. In total, 116 locations were sampled with one sample from the topsoil (0–50 cm) and a second sample from the subsoil (50–100 cm) (Figure 4.2). In addition to the point measurements, the LUCAS topsoil physical properties for Europe soil map [Ballabio *et al.*, 2016] and the European Soil Database (ESDB) derived data product [Hiederer, 2013] provide soil information for the area at a resolution of 500x500 and 1000x1000 m, respectively (Table 4.2). These data sources were combined to create soil texture (point measurements+LUCAS) and soil organic carbon (point measurements+ESDB) maps for model input (Figure 4.2). In a first step, for the unsampled regions, data points were extracted from the map products in a sampling density equal to the average density of the soil sampling locations (~580x580 m). Next, the extracted points were combined with the sampled points to a single set of data points (Figure 4.2). Then, the points were interpolated to the target resolution of 100x100 m using ordinary kriging and a spherical variogram model with a radius that included 30 measurements around an estimation point. Topographic information was available through the European Digital Elevation Model (EU-DEM) [Copernicus, 2016], version 1.1 at a spatial resolution of 25x25 m (Figure 4.1). Detailed maps of the

agricultural fields and orchards were provided by the Hellenic Payment and Control Agency for Guidance and Guarantee Community Aid while the land use of the remaining area was digitized from satellite imagery, using ArcGIS<sup>®</sup> software by Esri (Figure 4.1).

Orchard scale SM data were retrieved from S09 and S10, which were equipped for extensive monitoring in September 2020 (Figure 4.1). SM was monitored via a SoilNet wireless sensor network [Bogena *et al.*, 2010; Bogena *et al.*, 2022] with 12 nodes per orchard. Each node had six SMT100 SM sensors (Truebner GmbH, Neustadt, Germany) divided into two separate profiles which were installed at 5, 20, and 50 cm depth as well as two TEROS21 soil matric potential (SMP) sensors (METER Group Inc., Pullman, USA) installed at 20 cm depth. Irrigation amounts were recorded with TW-N flowmeters (TECNIDRO, Genova, Italy), installed at different irrigation sectors within the orchards. Meteorological data was collected by the cost-effective but reliable all-in-one ATMOS41 weather station (METER Group Inc., Pullman, USA) installed above the canopy in each orchard [Dombrowski *et al.*, 2021]. A more detailed description of the instrumentation and setup used to monitor SM dynamics, irrigation, and meteorological variables is given in Brogi *et al.* [2023]. Additionally, S10 was equipped with six SFM-1 sapflow sensors (ICT International Pty Ltd, Armidale, Australia) to estimate whole-tree transpiration. The sapflow sensors were installed on the trunk of six trees to represent, as much as possible, the orchards' trees in terms of height, perimeter, and vigor covering all five varieties. The installation and data correction followed the procedure outlined in Burgess [2018]. Phenology of the three main apple varieties was monitored using six phenocams (SnapShot Cloud 4G, Dörr GmbH, Germany) installed in S10.

Table 4.2: Main characteristics of the different soil data products used for the surface file creation of the regional case.

|                               | <b>European Soil Database Derived data</b>                                    | <b>LUCAS topsoil physical properties for Europe</b>     |
|-------------------------------|---|---|
| Underlying observational data | European Soil Database, Harmonized World Soil Database, Soil-Terrain Database | LUCAS 2009 soil survey (around 20 000 points) for EU-25 |
| Resolution (m)                | 1000x1000   | 500x500   |
| Soil texture                  | Yes   | Yes   |
| Organic matter                | Yes   | No  |
| Depth ranges (cm)             | 0–30, 30–100  | 0–20  |

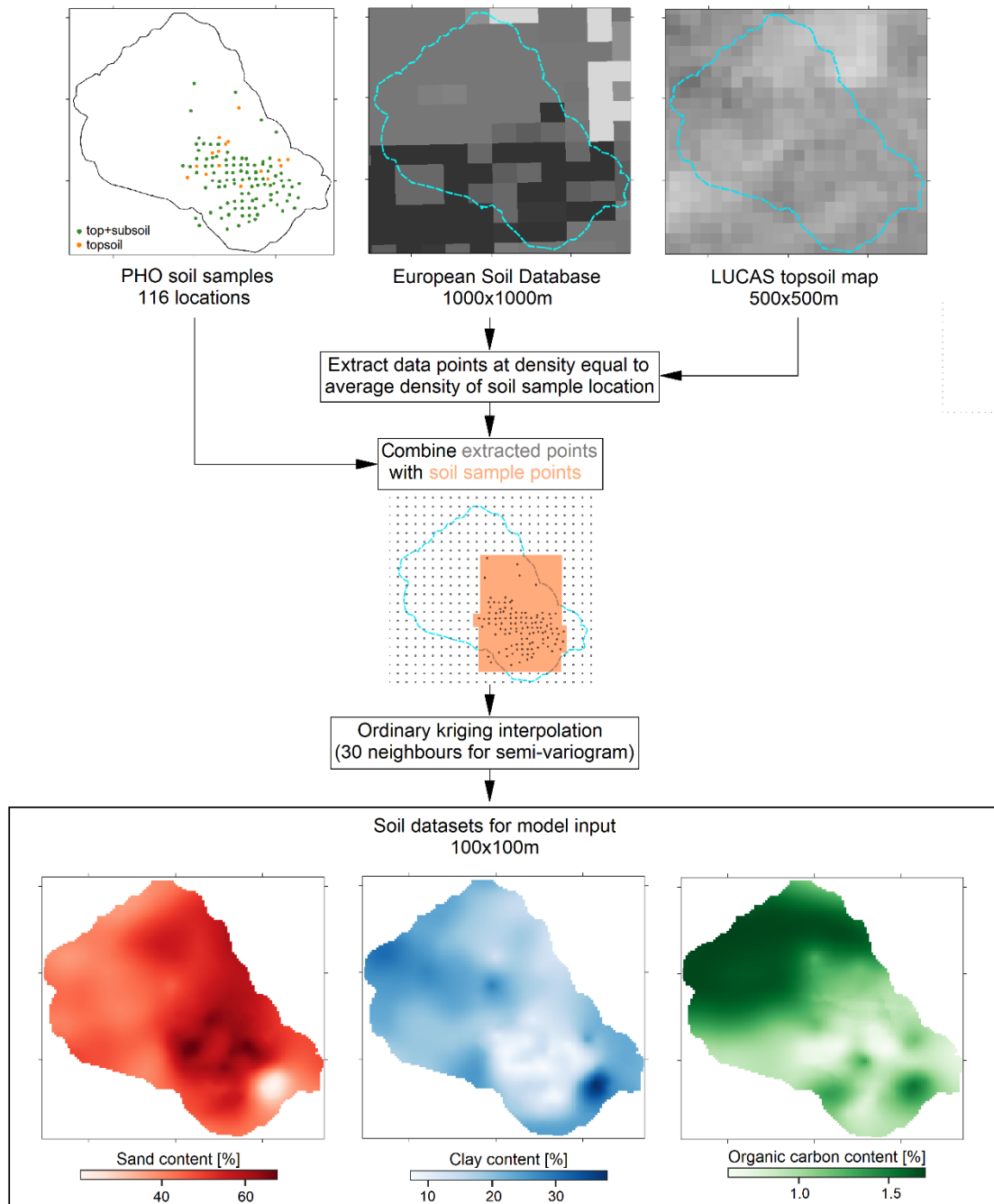


Figure 4.2 Top, from left to right: Soil sampling locations within the Pinios Hydrologic Observatory, soil data from the European soil database and the LUCAS topsoil map. Bottom: Soil texture input data sets of sand, clay, and organic carbon derived from the three data sources.

## 4.2.3 The land surface model

### 4.2.3.1 The Community Land Model

The Community Land Model v.5 (CLM5) used in this study is the latest version of the land component in the Community Earth System Model as described in detail by *Lawrence et al.* [2019]. CLM5 simulates land surface energy fluxes as well as

hydrological, biogeophysical, and biogeochemical processes that are driven by atmospheric input variables in combination with soil and vegetation states and characteristics [Lawrence *et al.*, 2018]. These processes are simulated on different subgrid units within a grid cell. Subgrid units include (1) the land unit defining the land use category (e.g., vegetated, urban, crop), (2) the column that is represented by 20 soil and 5 bedrock layers and resolves state variables and fluxes of water and energy in the soil, and (3) the patch level capturing biogeophysical and biogeochemical differences between plant functional types (PFTs) (e.g., broadleaf deciduous forest, evergreen shrub, maize, soy). The one-dimensional multilayer vertical water flow in the soil is simulated using a modified Richards equation [Dingman, 2015]. Soil hydraulic parameters for these calculations are derived from pedotransfer functions of sand and clay [Clapp and Hornberger, 1978; Cosby *et al.*, 1984] and organic properties of the soil [Lawrence and Slater, 2008]. With version 5 of CLM, a plant hydraulic stress routine was introduced that uses a simple hydraulic framework to model water transport along a water potential gradient from soil via plant to atmosphere [Kennedy *et al.*, 2019]. The new configuration replaces soil potential with leaf potential as the basis for plant water stress while root water potential is used to drive root water uptake. A new biogeochemistry and crop module, BGC-Crop, enhanced the representation of major crop functional types and land management practices such as irrigation and fertilization. Unlike natural vegetation that competes for water and nutrients, crops operate on separate soil columns that may be irrigated or non-irrigated, thus allowing for differences in land management [Lawrence *et al.*, 2019].

The recent development of CLM5-FruitTree enables the simulation of deciduous fruit trees and associated management practices in CLM5. The main features of the new sub-model include (1) a perennial phenology routine that allows the woody plant parts to remain on the orchard for several years, (2) carbon storage dynamics that enable the regrowth of annual plant parts, (3) an adapted carbon and nitrogen allocation, and (4) the description of typical management practices such as transplanting, pruning, and orchard rotation. Additionally, a new apple plant functional type was parameterized while fertilization and irrigation use the default CLM5 schemes. The complete model development of CLM5-FruitTree is described in Dombrowski *et al.* [2022].

### 4.2.3.2 Irrigation module in CLM5

Irrigation is performed individually over each irrigated soil column and responds dynamically to SM based on a daily check at 6 am. If crop leaf area is non-zero and if the available soil water over a specified irrigation depth  $z_{irrig}$  (=0.6 m by default) is below a defined threshold, irrigation is triggered. The irrigation amount is based on the SM deficit ( $D_{irrig}$ ) that is calculated over  $z_{irrig}$ :

$$D_{irrig} = w_{thresh} - w_{avail} \quad (4.1)$$

where  $w_{avail}$  is the available SM (mm) and  $w_{thresh}$  is the irrigation SM threshold (mm) calculated as:

$$w_{thresh} = f_{thresh}(w_{target} - w_{wilt}) + w_{wilt} \quad (4.2)$$

where  $w_{target}$  is the irrigation target SM (mm),  $w_{wilt}$  is the SM at wilting point (mm), and  $f_{thresh}$  is a tuning parameter. If  $f_{thresh} = 1$  (default), irrigation will be triggered once the available SM is below  $w_{target}$ . If  $f_{thresh} = 0$ , irrigation is only triggered once the available SM falls below  $w_{wilt}$ . Target SM is determined as the sum of SM at the target SM of each soil layer:

$$w_{target} = \sum_{i=1}^{n_{irr}} \theta_{target,i} * \Delta z_i \quad (4.3)$$

where  $n_{irr}$  is the index of the soil layer corresponding to  $z_{irrig}$ ,  $\Delta z_i$  (mm) is the depth of the soil layer  $i$  and  $\theta_{target,i}$  is the target volumetric SM value in a given soil layer. Similarly,  $w_{wilt}$  is calculated as the sum of SM at wilting point of each soil layer:

$$w_{wilt} = \sum_{i=1}^{n_{irr}} \theta_{wilt,i} * \Delta z_i \quad (4.4)$$

where  $\theta_{wilt,i}$  is the volumetric SM value at wilting point in a given soil layer.  $\theta_{target}$  and  $\theta_{wilt}$  are calculated by inverting the equation for soil matric potential (SMP) (Eq. 7.53 in Lawrence *et al.* [2018]) at the respective depth. By default, the SMP parameters  $\psi_{target}$  and  $\psi_{wilt}$  are set to  $-34$  and  $-1500$  kPa, considered field capacity and permanent wilting point, respectively.

In addition to  $w_{target}$ ,  $w_{wilt}$ ,  $f_{thresh}$ , and  $z_{irrig}$ , the user can define the irrigation duration ( $T_{irrig}$ ). Irrigation is applied directly to the ground surface at an intensity equal to  $\frac{D_{irrig}}{T_{irrig}}$ .

Irrigation parameters are not spatially distributed but are defined globally for a given model domain independent of geographic location or crop type.

### **4.2.3.3 Irrigation data stream implementation**

To study and evaluate the modelling outcomes under specific observed irrigation practices, an irrigation data stream was implemented in CLM5 to enable continuous prescription of irrigation parameters, i.e., irrigation rate, duration, and start time. These parameters are defined separately for one or multiple crop types and for each grid cell. This allows to account for differences in irrigation management depending on crop type and location to accurately reproduce local management practices. In addition, using the data stream, the applied irrigation amount can be easily adjusted, thus creating different irrigation scenarios while maintaining the same irrigation schedule. As irrigation is prescribed, the irrigation SM threshold that is calculated in the standard irrigation routine is not needed for this implementation.

## **4.2.4 Model implementation**

### **4.2.4.1 Orchard scale simulations**

For the simulations of S09 and S10, CLM5-FruitTree was run in single point mode and forced with hourly meteorological data from the two orchards. Fertilizer amount and soil texture were adjusted according to information provided by the farmer and soil samples. The default parameter file was adapted to account for the local climate and orchards characteristics. Crop parameters such as the different phenological stages were adjusted according to observations from the phenocam pictures, harvest information, and communication with the farmer. In the absence of observed bud break dates, parameters for the bud break prediction model were calibrated such that bud break would occur around the estimated date of 15<sup>th</sup> of March using the available local climate data. The modified crop parameters are listed in Table 4.3. Additionally, the observed irrigation time series was used as input to the irrigation data stream.

In order to balance ecosystem carbon and nitrogen pools and total water storage in CLM5 [Lawrence *et al.*, 2018], a 200 years model spin-up was performed. For this, the



CRUNCEPv7 atmospheric forcing data set from 1986 to 2016 [Viovy, 2018] and the parameterized apple plant functional type were used. Using the model state at the end of the spin-up, simulations were then re-initiated from planting in 2013 (S09) and 2015 (S10) using meteorological data from climate station CS1 (2016–2020) and data from the ATMOS41 sensors installed in the orchards for the years 2021 and 2022.

Table 4.3: Local crop parameters for the apple plant functional type.

| Parameter  | Variable name (unit)  | Value  |
|--|---|--------|
| Base temperature for bud burst prediction and GDD summation  | baset (°C)  | 8.5    |
| Chilling requirements for bud burst  | crequ (chill days)  | -126   |
| Critical temperature to initiate leaf offset   | crit_temp (K)   | 281.15 |
| Final root allocation coefficient until harvest  | arootf2 (unitless)  | 0.12   |
| GDD needed from bud break to canopy maturity   | lfmat (degree days)   | 1350   |
| GDD needed from bud break to harvest   | hybgdd (degree days)  | 2100   |
| GDD needed from bud break to the fruit ripening phase  | gnrp (degree days)  | 640    |
| GDD needed from bud break to the start of fruit development  | grnfill (degree days)   | 130    |
| Initial leaf allocation coefficient  | fleafi (unitless)   | 0.25   |
| Maximum canopy height  | ztopmx (m)  | 3.65   |
| Maximum harvest date in the northern hemisphere  | max_NH_harvest_date (mmdd)                                      | 1120   |
| Maximum LAI  | laimx (m <sup>2</sup> m <sup>-2</sup> )                         | 2.1    |
| Maximum rooting depth  | root_dmx (m)  | 0.6    |
| Planting density   | nstem (# m <sup>-2</sup> )                                      | 0.202  |
| Ratio of height: radius at breast height   | taper (unitless)  | 95     |
| The slope of the relationship between leaf N per unit area (gN/m <sup>2</sup> ) and Vcmax25top (umol CO <sub>2</sub> /m <sup>2</sup> /s) | s_vcad (μmol CO <sub>2</sub> s <sup>-1</sup> gN <sup>-1</sup> ) | 30     |

#### 4.2.4.2 Regional case simulations

A regional model domain, encompassing the entire PHO, was set up at a spatial resolution of 1 ha. This resolution was a compromise between accounting for the diverse, patchy landscape with small field and orchard sizes (from a few 100 m<sup>2</sup> to some hectares) and a reasonable computational effort. For the land use information, the database of agricultural fields and orchards was combined with the remaining land uses digitized from satellite imagery. Since CLM5 allows to define fractional land use in a single grid cell, the overall area of individual land use classes was still accurately represented.

The slope of the terrain was derived from the EU-DEM. Furthermore, the surface parameter defining the depth to bedrock was adjusted based on the minimum (0.27 m) and maximum (1.3 m) depths available to roots from the ESDB, which were linearly scaled by the slope. In the plain area, the value was set between 10 and 20 m to represent the thick alluvial deposits and prevailing free drainage conditions. Lastly, the maximum fractional saturated area ( $f_{max}$ ) that controls runoff generation was set to zero for all grid cells containing crops due to the deep groundwater table, gentle sloping in the plain, and assuming that there are no large saturated areas in the fields and orchards.  $f_{max}$  was set to 0.16 in the remaining areas of the catchment as extracted from the global data set. The adjusted parameters for apple were used as described in Section 4.2.4.1 while a separate parameter set was used for cherries to account for the earlier start of the growing season and harvest, and lower productivity as compared to apples. For the sake of consistency, parameters for winter wheat and potato were also modified based on *Boas et al.* [2021] with minor adjustments to growing seasons to account for the local climate [*Dercas et al.*, 2022; *FAO*, 2023].

For the model spin-up, the available global GSWP3 v1 atmospheric forcing data set providing data from 1901 to 2010 at a 3-hourly temporal and 0.5° spatial resolution was used [*Lange and Büchner*, 2020]. The model was spun-up for 720 years until equilibrium for soil carbon and nitrogen pools, soil water storage, and other ecosystem variables was reached for all land uses in the catchment. For the remaining simulations, the model was forced with a 7-year time series obtained from the observational data of meteorological stations CS1, CS2 (2016–2022), and CS3 (2018–2022) in the study area as well as from the two ATMOS41 stations in orchard S09 and S10 (2021–2022) (Figure 4.1). The data was spatially interpolated to the same resolution as the surface data using inverse distance weighting. The interpolation of precipitation and temperature included a weighting factor for elevation variation using a linear correlation between station elevation and mean annual station precipitation and temperature, respectively, as described in *Panagoulia* [1995]. Another short spin-up period of 3 years was performed as the orchards had just reached their maximum lifespan before orchard rotation is initiated and new seedlings need a couple of years to reach the full productivity level [*Dombrowski et al.*, 2022].

### 4.2.5 Simulation scenarios

To assess how well CLM5-FruitTree can represent SM dynamics and crop growth in the study area, 1D simulations were first performed in orchards S09 and S10 for the growing seasons 2021 and 2022. Two model set-ups were tested: the first used the default CLM5 irrigation routine with adapted parameterization to approximate the observed irrigation schedule, while the second was prescribed with the observed irrigation through the irrigation data stream. By directly applying irrigation water to the ground surface, CLM5 assumes an irrigation efficiency of 100% which is hardly achieved in sprinkler irrigation [Gilley and Watts, 1977]. For the irrigation data stream, we thus assumed that only 75% of the water volume measured by the hydrometers is reaching the ground surface while the rest is lost through evaporation from leaf surfaces, transpiration of the grass cover in the orchard alleys, and leakages in the piping system. Modelling results were compared to observed SM and tree transpiration at a daily time step as well as crop yield and development. Pearson's coefficient of correlation ( $r$ ), the root mean square error (RMSE) and the percent bias (%bias) were calculated for statistical model evaluation.

For the regional case, we conducted three simulation experiments to test different irrigation scenarios. Regional data on irrigation outside the instrumented orchards S09 and S10 was not available. Thus, the model was run using the default CLM5 irrigation routine with the same parameterization that was used for the point scale simulations, in the following considered the full irrigation scenario (FI). Based on this scenario, two deficit irrigation scenarios were created for both apple and cherry orchards with 75 and 50% of full irrigation (DI75 and DI50, respectively) using the irrigation data stream. All scenarios were run over the same 7-year period (2016–2022). To investigate the differences between irrigation scenarios, multi-year averages and seasonal dynamics of irrigation, SM, crop growth or yield, and crop water use efficiency (CWUE) were calculated and compared. In this study, CWUE was defined as the amount of yield produced per unit volume of water consumed [Ibragimov *et al.*, 2007]:

$$CWUE = \frac{Y}{ET} \quad (4.5)$$

where  $Y$  is crop yield in  $\text{t ha}^{-1}$  and  $ET$  is crop evapotranspiration in mm.

## 4.3 Results

### 4.3.1 Orchard scale simulations

#### 4.3.1.1 Soil moisture and matric potential dynamics

##### Outside the irrigation season

Figure 4.3 and Figure 4.4 show the SM time series at 5, 20, and 50 cm depth and SMP at 20 cm depth for S09 and S10, respectively. The interquartile range ( $Q_{25}-Q_{75}$ ), calculated from 24 measurements (12 nodes with two profiles each) for every depth, shows considerable variability in SM, especially in S10 and at 50 cm depth. This reflects the high heterogeneity of soil texture and gravel content that was observed during soil sampling. When comparing the observed SM dynamics in the two orchards, S09 showed 4–12 vol% higher SM on average compared to S10 throughout the measurement period. The soil textural analysis of both orchards clearly showed a higher clay and organic matter content, and lower gravel content in S09 compared to S10 (Table 4.1). Frequent rainfall during the winter months (631 and 606 mm in 2021 and 2022 respectively) kept the soil close to saturation with average SMP around  $-8.5$  kPa in both orchards. Starting in April the soil gradually became drier causing a steep decline in SMP to around  $-500$  kPa (S09) and  $-300$  to  $-400$  kPa (S10) by mid-May. The decline resulted from low rainfall amounts and increased evaporation demand along with water consumption from the grasses in the alleys and the fruit trees. In addition to the observations, the simulation results using both the standard CLM5 irrigation routine and the irrigation data stream are shown for the corresponding CLM5 soil layers in Figure 4.3 and Figure 4.4. Table 4.4 lists the model quality parameters used to evaluate the simulation results. The model simulations outside the irrigation season, using either irrigation approach, corresponded well to the observed SM in S09. However, in S10, CLM5 overestimated SM in the soil profile by on average 4.5–7.3 vol%. The observed differences in SM between both orchards were not captured by the model where SM values in S10 were only 1–2 vol% higher. In April and May, just before the start of the irrigation season, the simulations showed the strongest deviation from observed values for both orchards as the soil drying was much less pronounced in the simulations.

### Irrigation season

In 2021 and 2022, the farmer irrigated every 5–7 days starting mid-May through October. Irrigation amounts per event varied strongly and averaged 14 and 25 mm in S09 and S10 respectively (upper panel of Figure 4.3 and Figure 4.4). Irrigation increased SM by up to 10 vol% in the top 5 cm and about 5 vol% at 50 cm depth. To represent the observed irrigation schedule, the CLM5 irrigation routine can be adjusted in two ways, by (1) adapting  $\psi_{target}$  or (2) tuning the  $f_{thresh}$  parameter. Figure 4.5 shows the effect that different values of these two parameters have on several aspects of the simulated irrigation (e.g., start of irrigation period, number of irrigation events, irrigation frequency) as well as on SM and crop yield. In both cases, a lower parameter value results in a later onset of irrigation, fewer irrigation events and lower total irrigation amounts. However, the parameters have different effects on irrigation frequency, whereby smaller values of  $f_{thresh}$  result in less frequent irrigation events while the irrigation volume per event increases (Figure 4.5). Changing  $\psi_{target}$ , on the other hand, has little effect on the irrigation frequency and volume. SM in the upper 50 cm of soil increases with increasing values of both parameters. The increase is exponential for  $\psi_{target}$  with values ranging between 0.195 and 0.275 cm<sup>3</sup> cm<sup>-3</sup> and almost linear for  $f_{thresh}$  with a somewhat smaller range. Consequently, varying  $\psi_{target}$  has a more pronounced effect on yield compared to  $f_{thresh}$  for the investigated range of parameter values.

For the model run using the standard irrigation routine, we set  $f_{thresh}$  to 0.7 while leaving  $\psi_{target}$  at its default value of -34 kPa, which resulted in approximately weekly irrigation events of on average 26 mm per event, starting mid-May. This, however, could only partially reproduce the observed irrigation schedule and SM dynamics compared to using the irrigation data stream. Nevertheless, both irrigation approaches showed fluctuations of similar magnitude compared to the observed values in the upper soil. Less dynamics than observed were simulated at 50 cm depth for both irrigation approaches and both orchards. The wet bias in S10 was still persistent throughout the profile for the simulation using the irrigation data stream while simulated SM based on the default irrigation routine dropped to the range of observed values (Figure 4.4).

Simulated and observed total yearly irrigation were similar in S09 with the observed effective irrigation being 433 and 458 mm (75% of actual measured irrigation) and simulated amounts being 425 and 439 mm for 2021 and 2022, respectively. In S10,

observed effective irrigation amounts were considerably higher than in S09, which could be expected considering the lower observed SM in S10. Compared to the observed 706 and 586 mm, for 2021 and 2022, respectively, the model applied only 393 and 388 mm, which is a result of the simulated wet bias.

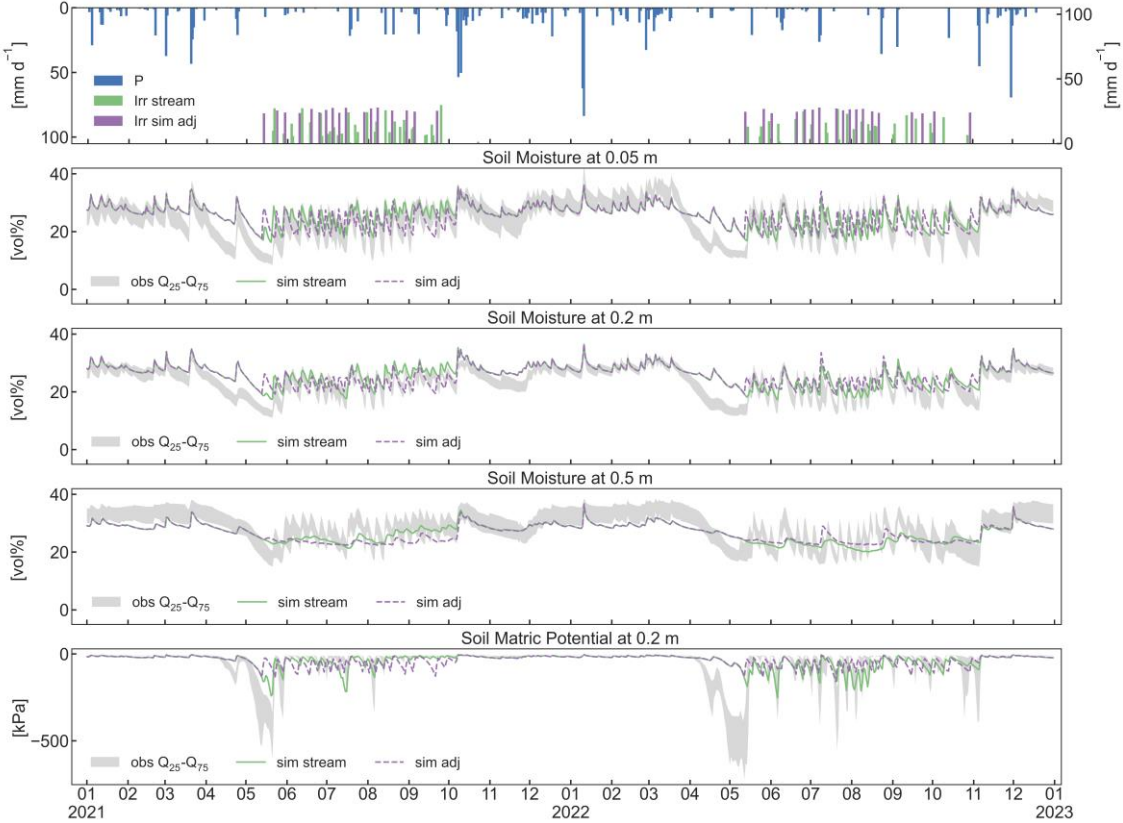


Figure 4.3 The upper panel shows precipitation, and observed and simulated irrigation for orchard S09 in mm d<sup>-1</sup>. The central panels show observed soil moisture (SM) as interquartile range between the 25<sup>th</sup> and the 75<sup>th</sup> percentile from 24 measurements, simulated SM using the standard CLM5 irrigation routine and the irrigation data stream at 5, 20, and 50 cm depths. The bottom panel shows observed interquartile range and simulations using the two irrigation approaches of soil matric potential (SMP) at 20 cm depth for orchard S09 for 2021 and 2022.

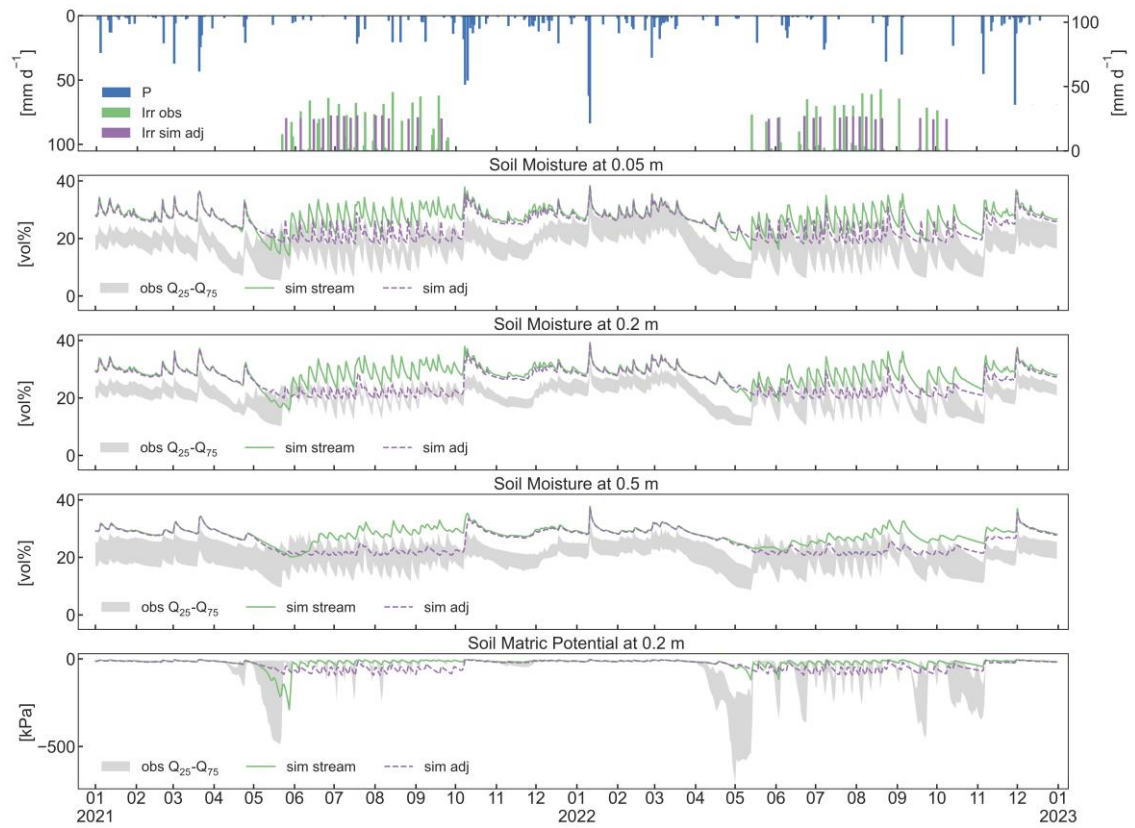


Figure 4.4 The upper panel shows precipitation, and observed and simulated irrigation for orchard S10 in  $\text{mm d}^{-1}$ . The central panels show observed soil moisture (SM) as interquartile range between the 25<sup>th</sup> and the 75<sup>th</sup> percentile from 24 measurements, simulated SM using the standard CLM5 irrigation routine and the irrigation data stream at 5, 20, and 50 cm depths. The bottom panel shows observed interquartile range and simulations using the two irrigation approaches of soil matric potential (SMP) at 20 cm depth for orchard S10 for 2021 and 2022.

Table 4.4: Pearson's coefficient of correlation ( $r$ ), root mean square error (RMSE) and percent bias (%bias) for soil moisture (SM) at 5, 20 and 50 cm depth and soil matric potential (SMP) at 20 cm depth in orchards S09 and S10 simulated using the irrigation data stream. The first number refers to 2021 and the second number to 2022. Statistics were calculated for the whole year and for the irrigation season only (21<sup>th</sup> May to 25<sup>th</sup> Sep for 2021; 15<sup>th</sup> May to 10<sup>th</sup> Oct and 14<sup>th</sup> May to 2<sup>nd</sup> Oct for S09 and S10, respectively, in 2022).

|                   |                | S09       |             |             | S10               |             |              |                   |
|-------------------|----------------|-----------|-------------|-------------|-------------------|-------------|--------------|-------------------|
|                   | Soil depth (m) | r         | RMSE (vol%) | %bias       | r                 | RMSE (vol%) | %bias        |                   |
| Whole year        | 2021/2022      | 0.05      | 0.88/0.81   | 3.97/3.89   | 13.13/8.18        | 0.77/0.83   | 9.55/8.08    | 50.21/39.89       |
|                   |                | 0.2       | 0.88/0.86   | 3.10/3.23   | 10.14/9.26        | 0.75/0.84   | 8.18/7.68    | 37.30/35.55       |
|                   |                | 0.5       | 0.78/0.80   | 3.08/3.49   | -6.60/-6.63       | 0.56/0.72   | 8.06/7.65    | 37.48/36.13       |
|                   |                | SMP (kPa) | 0.82/0.63   | 56.25/89.67 | -27.54/<br>-37.14 | 0.62/0.75   | 41.65/122.41 | -35.44/<br>-76.14 |
| Irrigation season | 2021/2022      | 0.05      | 0.86/0.74   | 3.85/3.02   | 15.47/4.30        | 0.70/0.83   | 5.13/8.43    | 21.13/45.60       |
|                   |                | 0.2       | 0.84/0.77   | 3.00/2.84   | 10.86/8.10        | 0.67/0.77   | 2.3/7.70     | 4.51/37.32        |
|                   |                | 0.5       | 0.48/0.27   | 3.12/3.74   | -6.27/-6.14       | 0.25/0.45   | 1.73/7.10    | -0.74/33.74       |
|                   |                | SMP (kPa) | 0.73/0.64   | 46.61/61.36 | -11.08/<br>-7.54  | 0.65/0.66   | 52.04/98.86  | -81.11/<br>-72.95 |



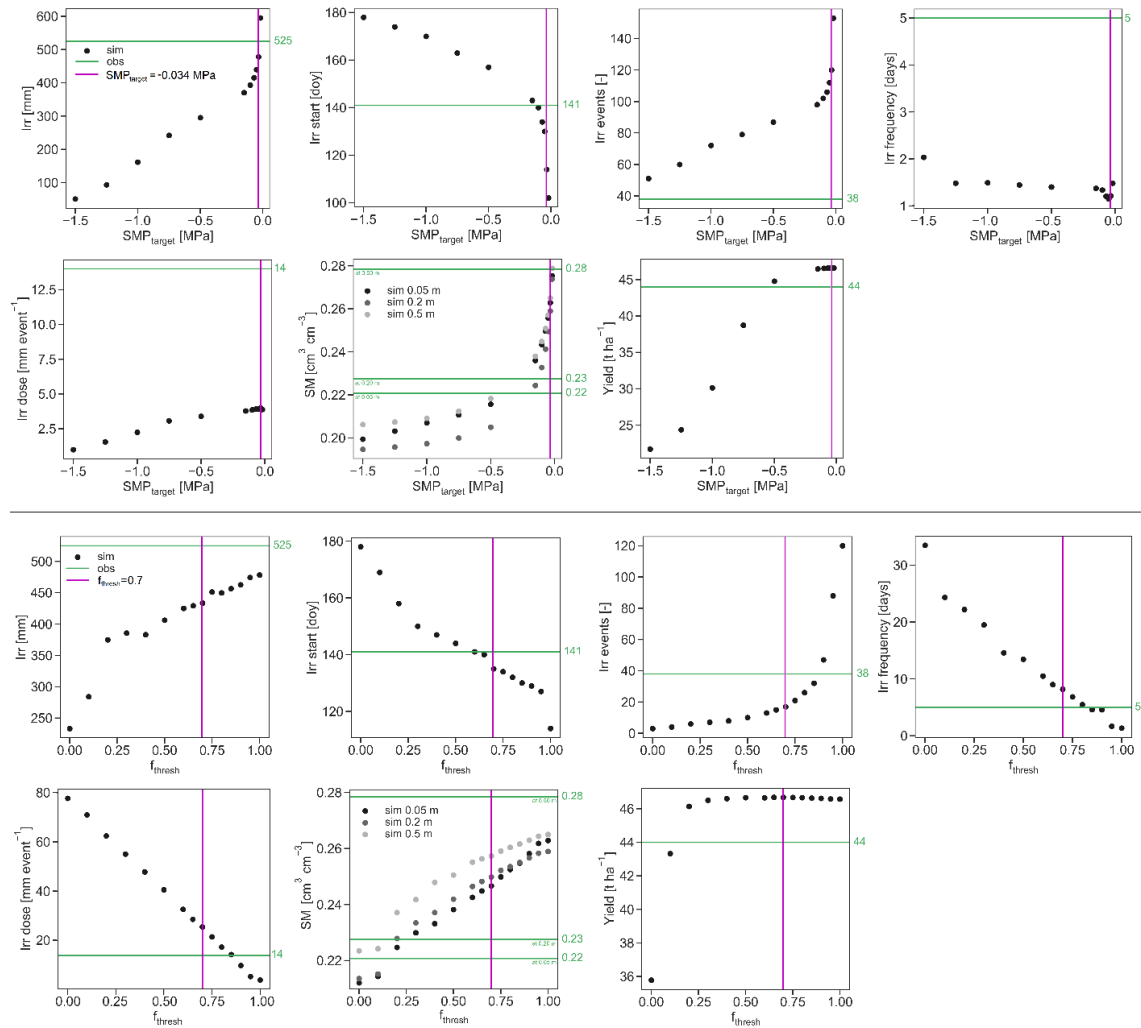


Figure 4.5 Effect of irrigation target soil matric potential ( $\psi_{target}$ ) and irrigation threshold fraction ( $f_{thresh}$ ) on total irrigation amount (Irr), irrigation starting date (Irr start), number of irrigation events (Irr events), irrigation frequency (Irr frequency), irrigation dose per event (Irr dose), soil moisture (SM) at 5, 20, and 50 cm depth, and yield. Shown are yearly average values for S09 and the year 2016.

#### 4.3.1.2 Tree transpiration and fruit harvest

The comparison of measured sapflow with simulated transpiration expressed as water consumption per tree is presented in Figure 4.6. Observed sapflow varied significantly between different trees resulting in large inter-quartile ranges. The two model runs showed no difference in simulated tree transpiration despite the difference in irrigation amount and timing. In 2021, CLM5 showed higher values and a slight shift in the seasonal dynamic as a result of a too early onset of leaf development compared to the observed values ( $LAI_{sim}$  in Figure 4.6). Simulated leaf duration and total transpiration agreed well with the measurements in 2022. Tree transpiration peaked in July with a measured monthly average of 12.5 (2021) and 20.2  $L\ tree^{-1}\ day^{-1}$  (2022) and simulated values of 25.1 (2021) and 24.5  $L\ tree^{-1}\ day^{-1}$  (2022). The better agreement between simulated and

observed values in 2022 followed a reinstallation that was performed after partial sensor failure and unreliable measurements that resulted in data gaps for the 2021 growing season. The 2021 data should therefore be handled with care when interpreting absolute values. Simulated maximum leaf area index (LAI) was reached in early July. Full canopy cover in the orchards occurred in the second half of June, so slightly earlier, based on visual inspection of the phenocam pictures (data not shown). Simulated leaf area and hence transpiration fell to zero by December, which broadly agreed with observed sapflow and leaf senescence deduced from the phenocam images.

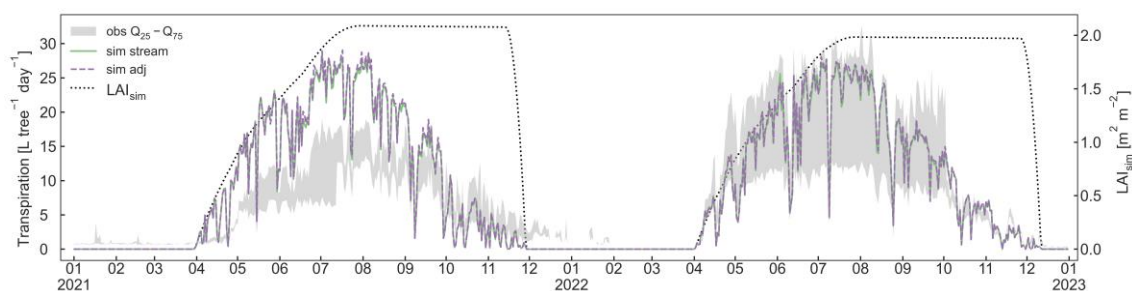


Figure 4.6 Whole tree transpiration estimated from the sapflow sensors in orchard S10 together with simulated transpiration expressed in liters per tree and day, and simulated leaf area index ( $LAI_{sim}$ ) for 2021 and 2022.

Generally, fruit harvest in the orchards was performed between 17<sup>th</sup> of August and 30<sup>th</sup> of October in a first and second harvest for most varieties. Due to very low apple quantity, harvest in 2022 occurred in a single harvest between 1<sup>st</sup> Sep and 15<sup>th</sup> Nov depending on variety. Simulated harvest in 2021 occurred on 12<sup>th</sup> and 18<sup>th</sup> Sep for S09 and S10 respectively, and a few days earlier in 2022. The two simulation runs using either the adapted CLM5 irrigation routine or the irrigation data stream showed no difference in harvest amounts. In 2021, simulated yield was close to the observed values while the exceptionally low yield in 2022 was not captured by the simulations (Table 4.5). Visual inspection of the phenocam images showed significantly less flowers on the trees in 2022 compared to 2021 (data not shown). No extreme weather conditions were observed during the winter 2021/2022 that could explain the reduced flowering. Other possible reasons for the low number of flowers and hence low yield in this year may be related to alternate bearing of the varieties or other factors (e.g., plant physiology or traits, pest and disease or certain management practices) that are not included in the model.

Table 4.5: Observed and simulated apple yield in  $\text{t ha}^{-1}$  for orchards S09 and S10 for 2021 and 2022.

| Year | Yield in S09 ( $\text{t ha}^{-1}$ ) |     | Yield in S10 ( $\text{t ha}^{-1}$ ) |     |
|------|-------------------------------------|-----|-------------------------------------|-----|
|      | obs                                 | sim | obs                                 | sim |
| 2021 | 44                                  | 47  | 47                                  | 51  |
| 2022 | 16                                  | 49  | 11                                  | 50  |

## 4.3.2 Regional simulations

### 4.3.2.1 Irrigation signature in the PHO

Figure 4.7 shows simulated seasonal mean SM and sum of evapotranspiration (ET) within the PHO averaged over the 7-year period. Depicted values represent grid cell averages, meaning they are the weighted average of all land uses in a given cell. During the winter months and into spring, SM is high throughout the catchment, but with a declining gradient along the North-South axis from the mountainous part down to the plain. ET in the catchment is low during winter but starts to increase in spring, revealing a discernible pattern attributed to differences in land use (Figure 4.1). During the summer months, ET reaches its peak, displaying a distinct irrigation signature with significantly higher ET values of 293 mm on average over irrigated land, as opposed to 214 mm on average in the rest of the catchment. The pattern persists throughout autumn and is also evident in summer and autumn SM, albeit less pronounced due to the lower productivity of rainfed vegetation, resulting in reduced water uptake from the soil. The subsequent analysis will focus exclusively on the irrigated land, more specifically on apple orchards, as they account for 91% of the total irrigated area.

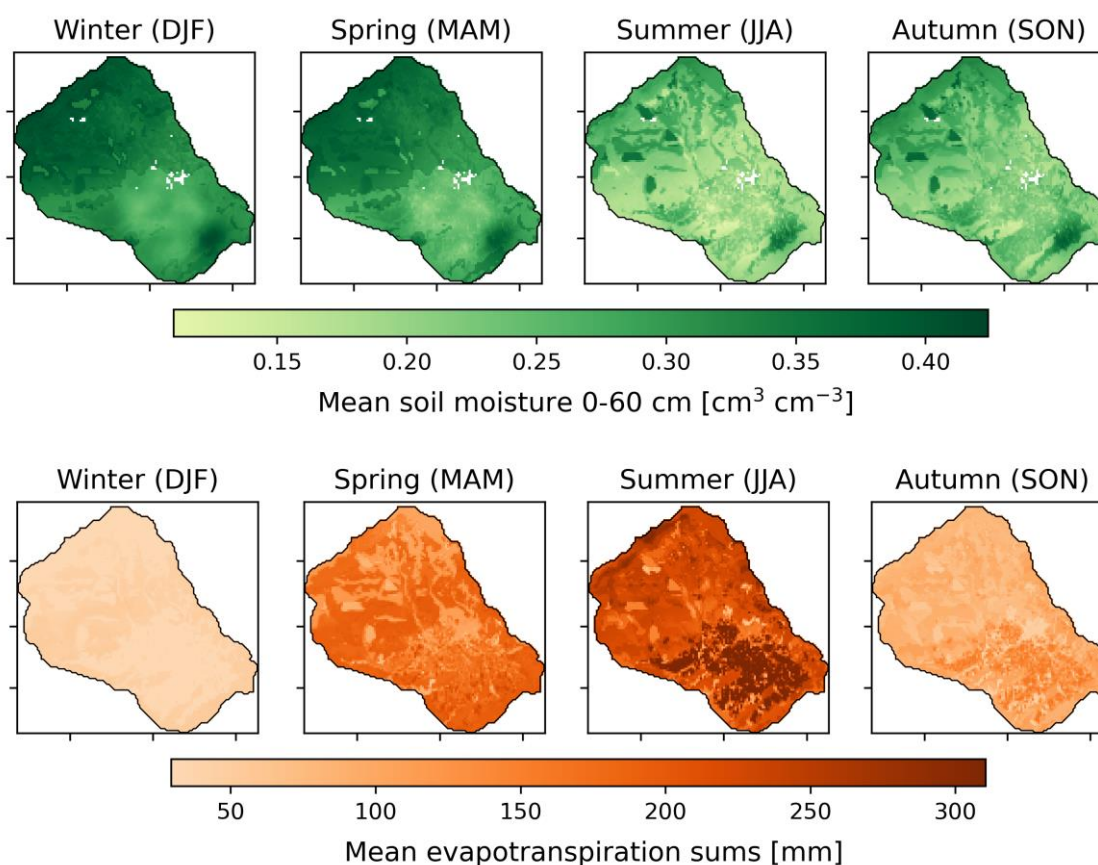


Figure 4.7 Seasonal mean soil moisture, and evapotranspiration sums in the PHO catchment, averaged over the period 2016–2022.

#### 4.3.2.2 Simulated spatial patterns

Figure 4.8 shows average and standard deviation of the 7-year simulation period for irrigation, SM, yield, and CWUE for all apple orchards in the PHO, between 2016 and 2022. Modelling results show a clear spatial pattern that is driven by climatic conditions following the topographic gradient (Figure 4.1) on the one hand and soil characteristics on the other hand (Figure 4.2). Average yearly irrigation requirements range between 400 and 450 mm in the plain. The highest values are found in the southeast while considerably lower values occur at higher altitudes in the northern part of the catchment ( $< 200$  mm). Harvest values show a similar pattern because cooler temperatures and lower incoming radiation in the northern part of the catchment result in lower crop productivity and thus smaller yields ( $16\text{--}38 \text{ t ha}^{-1}$ ) compared to the plain where yields are around  $50 \text{ t ha}^{-1}$  without much spatial variability. In addition to lower crop productivity and thus lower crop water demands, spatial variability in irrigation requirements results from the higher precipitation in the upper parts of the catchment that further reduces the need for irrigation as well as soil textural differences. The latter is most evident in the southern part of the catchment where the higher clay content and the consequently higher water holding

capacity of the soil result in increased evaporation (not shown). This in turn generates a greater irrigation demand resulting in slightly lower CWUE of orchards planted on these soils. Soil textural differences are also reflected in the SM plot where areas with a higher percentage of clay or organic matter show higher SM values than areas with sandier soils or soils that are lower in organic matter. CWUE ranges from 57–65  $\text{kg ha}^{-1} \text{mm}^{-1}$  in the plain to 35–45  $\text{kg ha}^{-1} \text{mm}^{-1}$  in the northern part of the catchment and largely reflects the spatial patterns of irrigation and harvest whereby high irrigation requirements and low harvest lead to low CWUE. Inter-annual variability (standard deviation plots) within the catchment shows similar patterns for irrigation, harvest, and CWUE and is higher in the northwestern part of the catchment. The higher variability was driven by local temperature differences in some years that delayed the onset of the growing season up to 14 days compared to the remaining orchards. Inter-annual variability of SM is generally low without a distinct spatial pattern.

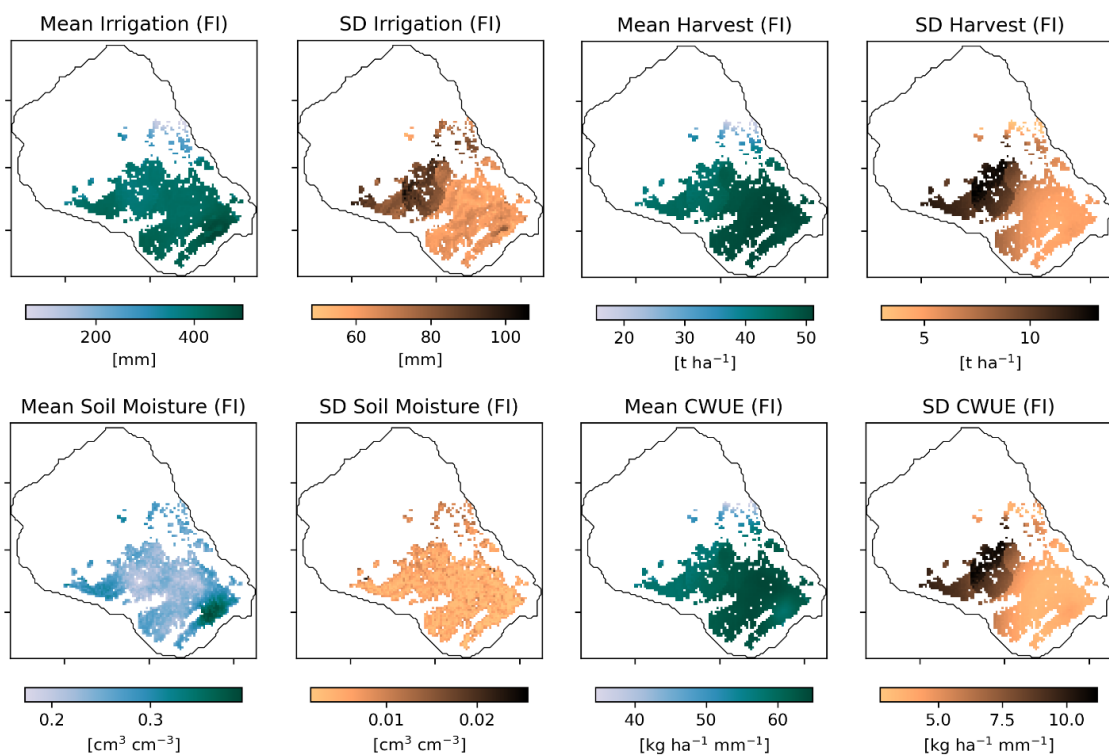


Figure 4.8 Mean and standard deviation (SD) of average yearly irrigation, soil moisture in the root zone (0–60 cm), harvest, and crop water use efficiency (CWUE) for apple orchards within the PHO between 2016–2022 under full irrigation (FI).

### 4.3.2.3 Effect of irrigation deficit scenarios

The effect of deficit irrigation on total irrigation amounts, harvest, and CWUE of apple orchards in the PHO for the moderate irrigation deficit scenario, DI75, and the more severe deficit scenario, DI50, are shown in Figure 4.9. Yield differences between the FI and the DI75 scenario are almost negligible, ranging from a decline of maximum 3 t ha<sup>-1</sup> (5%) to even slight increases in yield. However, the DI50 scenario resulted in a clear decline of simulated yield with up to 12 t ha<sup>-1</sup> corresponding to a 30% reduction in yield compared to the FI scenario. Nonetheless, orchards located at high altitudes and in the southeast on clay-rich soils are still barely affected by the higher water deficit (< 5% decline in yield). Overall, annual water savings are highest in the plain, averaging 100–125 mm for DI75 and 210–250 mm for DI50. CWUE shows a differing pattern between both scenarios. While in DI75, CWUE declines slightly in the central part of the plain by around 1 kg ha<sup>-1</sup> mm<sup>-1</sup> (2%), there are large areas that show an increase in CWUE of similar magnitude. The decline in CWUE is concentrated on the orchards growing on soils with a high percentage of sand. For DI50, on the other hand, CWUE is almost exclusively showing a decrease of up to 8.8 kg ha<sup>-1</sup> mm<sup>-1</sup> (17%), though again CWUE for orchards in the higher altitudes and the ones located on soils with higher clay content are less affected.

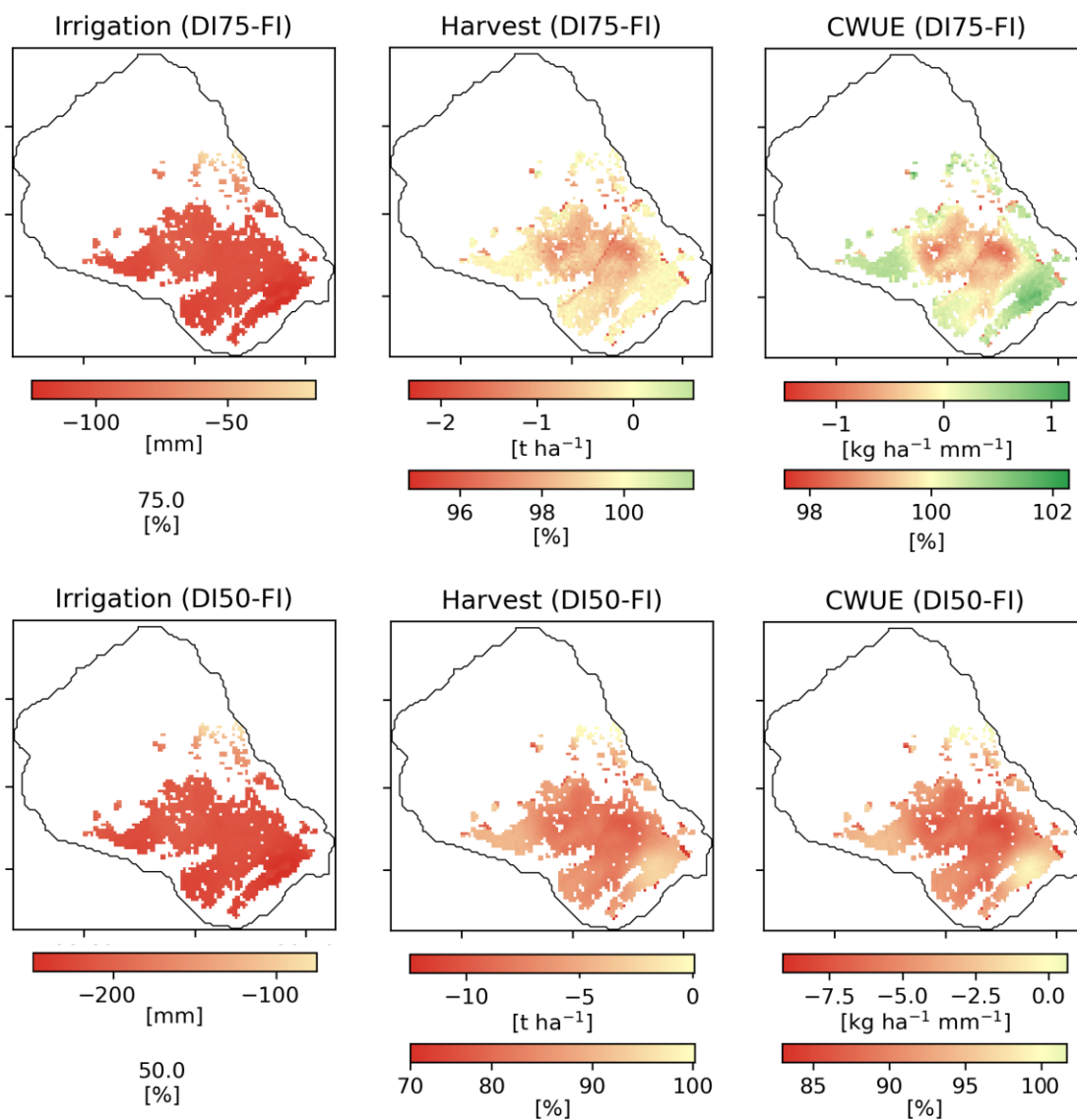


Figure 4.9 Absolute and relative differences in irrigation amount, harvest, and crop water use efficiency (CWUE) between the full and the 75% irrigation scenario (DI75-FI), and the full and 50% irrigation scenario (DI50-FI) for apple orchards within the PHO during the period 2016–2022.

#### 4.3.2.4 Irrigation and yield at the inter-annual and monthly scale

Yearly irrigation amounts, precipitation during the main irrigation season, and harvest averaged for all apple orchards in the PHO are shown in Figure 4.10. For the investigated 7-year period, irrigation ranges between 297 and 487 mm while precipitation is around 167–322 mm from May to October. Differences in precipitation drive the inter-annual variability in irrigation requirements whereby drier summer months, such as 2019–2022, result in higher irrigation demand compared to wetter years. Yield ranges between 32 and 55 t ha<sup>-1</sup>, with 2019 and 2020 being the years with the highest yields due to favourable meteorological conditions (high solar radiation and temperature). Notably, the effect of deficit irrigation on yield is strongest in these two years reducing yield by > 12 t ha<sup>-1</sup> for the DI50 scenario. In contrast, both the DI75 and DI50 scenario have negligible effect on yield in the first three simulation years.

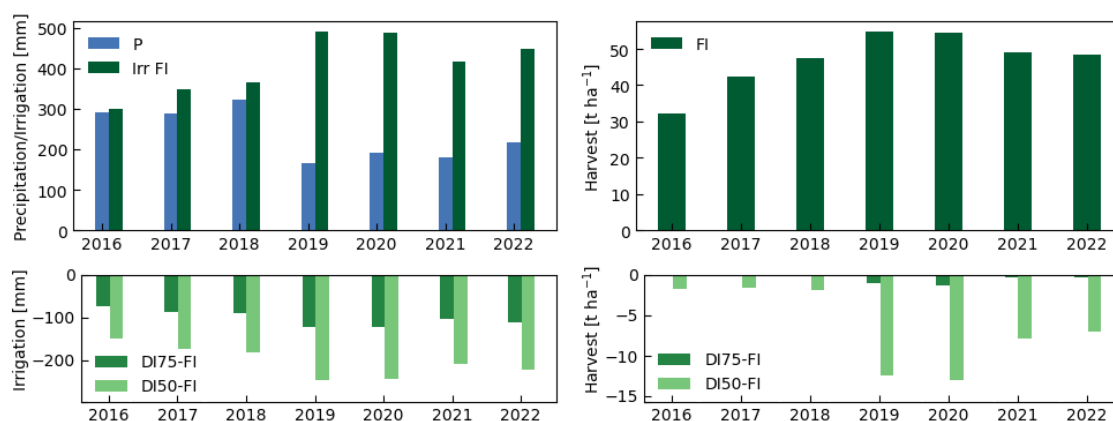


Figure 4.10 Yearly sum of precipitation during the main irrigation season (May-Oct), irrigation, and harvest averaged over all apple orchards within the PHO from 2016 to 2022, under full irrigation (FI) and the difference for the 75% and the 50% deficit irrigation scenarios (DI75 and DI50).

Figure 4.11 shows the seasonal course of irrigation, precipitation, and fruit growth in the apple orchards averaged over the PHO and the 7-year period. The simulated irrigation season starts in April or May and lasts until October with negligible amounts still applied in November for some years. Monthly irrigation requirements increase sharply between April and June until reaching their peak in August with on average 107 mm per month. Accordingly, August is also the month in which the greatest water savings occur for the deficit scenarios. After that, irrigation declines rapidly. Fruit biomass increases steadily from April to harvest in September with faster growth occurring in the earlier months. While fruit growth is barely affected by a 25% reduction in irrigation (DI75), for the DI50 scenario it decreases sharply in August and to a smaller extent in July and September.



The reduced fruit growth results in a yield loss of on average 0.5 t ha<sup>-1</sup> for DI75 and 6.5 t ha<sup>-1</sup> for DI50.

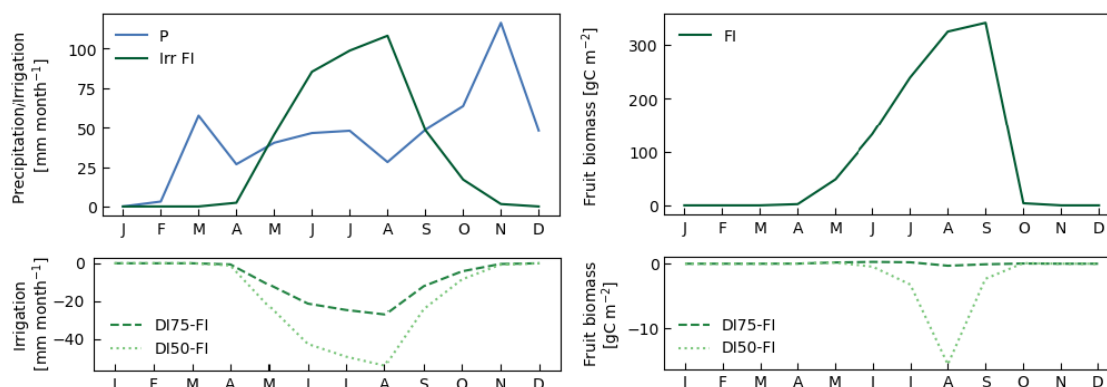


Figure 4.11 Seasonal pattern of monthly precipitation, irrigation, and fruit biomass averaged over all apple orchards within the PHO and the period 2016–2022, under full irrigation (FI) and the difference for the 75% and the 50% deficit irrigation scenarios (DI75 and DI50).

## 4.4 Discussion

### 4.4.1 Evaluation of the CLM5 irrigation routine

The direct comparison of simulated SM dynamics to observed SM from a dense sensor network in two irrigated orchards gave valuable insights into model performance. Our findings demonstrate that the standard CLM5 irrigation routine lacks the necessary flexibility to represent specific irrigation practices observed in the orchards. Simulated crop growth and transpiration at the orchard scale were not sensitive to the difference in irrigation amount and timing between the two model runs using the standard irrigation routine and the implemented irrigation data stream respectively. However, as differences between the simulated and actual irrigation practices increase, the effects may become more important especially considering runoff generation or sensible and latent heat fluxes that were not analysed in this study. Similarly, if the irrigation is limited so that the crop experiences some degree of water stress, the timing of irrigation may become more important. This could be further tested by applying different irrigation schedules under various amounts of irrigation using the irrigation data stream.

Prior studies using the irrigation module in CLM were limited to calibrating the target SM or adjusting the irrigation threshold fraction to match gross irrigation requirements reported at the country or regional level, or performed no calibration at all [Felfelani *et al.*, 2018; Leng *et al.*, 2015; Leng *et al.*, 2013; Zhu *et al.*, 2020]. The model, however,

does not currently consider restrictions on irrigation schedule, over irrigation, or irrigation efficiency that significantly affect gross irrigation requirements as our results revealed. The newly implemented irrigation data stream can be used to overcome some of these limitations by prescribing crop and farmer specific irrigation schedules and amounts. This allows investigating the irrigation-induced effects on e.g., crop yield, SM, or carbon and energy fluxes under observed irrigation practices and can help to identify existing model biases by removing one possible source of uncertainty. While the use of the irrigation data stream at larger scale is currently hampered by the limited availability of precise information on irrigation practices in most areas [Felfelani *et al.*, 2018], it can serve as a valuable tool to investigate the modelled effect of different irrigation schedules and water availability scenarios. This can offer a basis and direction for further developments of the irrigation routine that are necessary for a more realistic representation of irrigation management practices [Yao *et al.*, 2022].

## **4.4.2 Model uncertainties and limitations of this study**

### **4.4.2.1 Parametric uncertainty**

SM dynamics outside the growing season were well reproduced by CLM5, indicating that the model was able to capture infiltration and soil water redistribution in the studied orchards. However, the significant SM bias in S10 suggests structural and parametric uncertainty in the estimation of soil hydraulic properties, probably due to inappropriate pedotransfer functions implemented in CLM5 [Han *et al.*, 2015]. Gao *et al.* [2021] found that poor performance of CLM5 in reproducing observed root zone SM was mainly due to uncertainty in porosity estimates. In addition, a high content of rock fragments, which is typical of many Mediterranean soils [Nijland *et al.*, 2010; Poesen and Lavee, 1994; Zilidis *et al.*, 2002], can strongly influence the SM regime through non-linearity in soil hydraulic conductivity and by reducing the soils' effective porosity [Angulo-Jaramillo *et al.*, 1997]. For this reason, most pedotransfer functions fail to correctly reproduce the hydraulic properties of stony soils [Nasri *et al.*, 2015], which likely led to biases in simulated SM in S10. Further investigation of the results would be needed to confirm this hypothesis, e.g. data assimilation of observed soil variables could be used to optimize soil hydraulic parameters [Strebel *et al.*, 2022]. In both orchards, the simulations showed a lower simulated SM dynamic in 50 cm depth, which could be the result of uncertainties in the rooting distribution and thus root water uptake within the soil profile. The current

parameterization of the vertical discretization of root fraction results in a rather shallow profile while deeper roots may still contribute to root water uptake in the studied orchards. *Shrestha et al.* [2018] encountered a similar issue when analyzing root zone SM on a grassland site using CLM3.5 and were able to improve simulated SM dynamics by increasing the root fraction in deeper layers. This may help to improve the simulated SM dynamics at 50 cm on our study sites.

The sensitivity experiments performed using two parameters of the CLM5 irrigation routine (Figure 4.5) and the results from the irrigation scenarios revealed relatively low sensitivity of crop yield to reduced irrigation (Figure 4.9). The new plant hydraulics introduced by *Kennedy et al.* [2019] advanced the physical basis for hydraulic stress in the model, but there is large uncertainty in its parameterization and in capturing the relationship of plant water stress and SM deficit for different crops. To better quantify the model performance and find the most suitable parameters for apple orchards, comparison of simulations to observations from stressed and non-stressed crops would be necessary. Additionally, sensitivity analysis of plant hydraulic parameters, which was out of the scope for this paper, could help to better constrain these model parameters.

#### 4.4.2.2 Crop representation

The PHO catchment is characterized by a diversity of small-scale farm holders resulting in considerable heterogeneity in management practices, which cannot be fully captured by the model. While simulated yield was close to observations during a “good” year for the point-scale simulations, according to *Mattas et al.* [2019] average Greek apple production in 2016 was only  $\sim 23 \text{ t ha}^{-1}$ . This suggests a great variability in orchard productivity, apple cultivars, or type of end product (e.g. apples for direct consumption or for juice) which would necessitate the inclusion of additional crop types and management practices in CLM5. In striving for global applicability, CLM5 and other LSMs face constraints in computational resources and often insufficient observational data to parameterize additional crop types, which results in biases in certain regions, while others are more accurately represented [*Lombardozzi et al.*, 2020]. In our case, the model demonstrated a strong correlation of yield and irrigation with the climatic gradient induced by the topography in the PHO, indicating a high sensitivity to model forcing data. The large simulated differences in yield between orchards in the plain ( $\sim 50 \text{ ton ha}^{-1}$ ) vs. the higher altitudes (as low as  $16 \text{ ton ha}^{-1}$ ) may however be exacerbated, as CLM5

employs a single set of parameters for a given crop across diverse geographies and climates. In reality, various cultivars of the same crop type, along with plant physiological adaptations to their environments, can lead to comparable productivity levels despite variations in climatic conditions. This phenomenon is evident in the cultivation of numerous crops, including apples, across climates on a global scale [Sherman and Beckman, 2002]. The issue has been addressed by Lombardozzi *et al.* [2020] who recommended further developments in CLM5 to improve phenological triggers and agricultural management, and to include different cultivars. In the future, the incorporation of additional satellite-derived crop data, advanced parameterizations, or the use of crop calendars to constrain these models may help reduce some of the biases [Pongratz *et al.*, 2018; Yao *et al.*, 2022; Zhang *et al.*, 2020].

At the orchard scale, we found discrepancies between observed and simulated SM during the growing season that suggest limitations specific to the current representation of orchards. As CLM5 does not allow intercropping, the actively growing grass cover in the orchard alleys is not included in the CLM5-FruitTree sub-model [Dombrowski *et al.*, 2022]. Consequently, our simulations do not account for the additional root water uptake and transpiration as well as interception of the irrigation water from the grasses. The former may explain the smaller simulated decline in SM early in the season compared to the observations, while we considered the latter to some extent by assuming a reduced irrigation efficiency. In doing so, we did however neglect the additional ET flux. Yao *et al.* [2022] developed and tested different irrigation techniques in CLM5 and found an increase in canopy evaporation through increased interception for their implementation of sprinkler irrigation. However, the overall impact on ET and total applied irrigation remained small compared to the control run using the standard CLM5 irrigation. More importantly, accounting for conveyance and application losses would increase the simulated irrigation amount and could lead to more realistic irrigation values [Yao *et al.*, 2022].

Despite these limitations, and though we could not validate the simulation of crop yield and irrigation requirements in the PHO catchment due to the lack of observational data, the reasonable modelling results at the orchard scale give some confidence in the robustness of the regional simulations.

### 4.4.3 Implications for irrigation management

We studied the relationship between crop yield and water use efficiency, and irrigation at the regional scale, as it is determinant for a reasonable allocation of irrigation water according to crop needs. For most part of the PHO, CWUE and yield were little affected when irrigation was reduced to 75%, suggesting that this scenario lies closer to the optimal irrigation that maximizes yield while minimizing water consumption as opposed to the FI scenario. These results are similar to a study by *Li et al.* [2018] who used CLM to schedule irrigation in a citrus orchard in Spain which resulted in 24% less irrigation compared to the farmers' practices. This could indicate that farmers irrigate too much when water is available and water prices are low [*Latinopoulos, 2005*]. Simulated apple yield was sensitive to a reduction of 50% of the applied irrigation water causing up to 30% decline in yields. The effect, however, varied with different meteorological conditions and soil types within the PHO. At higher altitudes, cooler temperatures and lower incoming radiation rather than water scarcity limited crop growth. Irrigation in these orchards could thus be greatly reduced without negatively affecting yield. Moreover, under the same climatic conditions, orchards growing on soils with a higher percentage of clay (southeastern part of the catchment) could maintain similar yield and CWUE under 50% reduction in irrigation water because of the greater water holding capacity of the soil. This will make orchards growing on these soils less prone to experience water stress. The effect of deficit irrigation on fruit growth and yield varied between years and throughout the growing season. Years with high productivity and greater dependence on irrigation (due to low rainfall) showed greater yield loss under deficit irrigation (Figure 4.10). At the seasonal scale, fruit growth showed the highest reduction in August followed by July and September (Figure 4.11). This was mainly an effect of higher temperature, little rainfall, and larger leaf area that resulted in high irrigation requirements in this month. Apples, similarly to other crops, show different susceptibility to drought stress depending on their growth stages whereby flowering and fruit set as well as fruit development and maturation are highly susceptible to drought. The latter stage falls within the period July to September where the model showed the largest reduction in fruit growth. While the simulated plant water stress is currently linked to environmental conditions rather than capturing plant physiological differences in this stage of growth, it suggests that under limited water conditions, irrigation should be prioritized during these months to maintain reasonable yields.

#### **4.4.4 Perspectives for further application and model development**

The analysis performed in this study displays the current ability and potential way forward of applying CLM5 for irrigation and water resources management at various scales. Prospectively, future applications and research studies should focus on the improvement of input data sets, crop and irrigation parameterizations, and process representation. Input related improvements include the creation of high-resolution climate and land use information, especially crop types and the extent and type of irrigation. Our results clearly showed how climate and environmental heterogeneity (e.g., topography, land use, soil properties) can greatly affect total crop water requirements, emphasizing the need for spatially explicit modelling for large-scale applications. Model investigation at the orchard scale revealed the importance of soil and crop-specific parameterization to correctly represent SM and phenology dynamics, and harvest time. Extending simulations to larger scales will thus require further improving soil hydraulic parameterization through improved pedotransfer functions [Vereecken *et al.*, 2022] or parametrization of soil hydraulic properties through data assimilation approaches [Han *et al.*, 2014]. Furthermore, information on crop management and improved differentiation between different crop varieties and cultivars (e.g. different growing seasons and harvest of cherry compared to apple trees) is necessary, as these can result in distinct irrigation seasons and amounts. Concerning irrigation, this could include either crop-specific or spatially explicit values for irrigation parameters that are currently the same for all irrigated crops, hence not reflecting different management strategies or susceptibilities to water stress. Lastly, some processes could be refined or added to represent irrigation requirements more realistically. These include a parameterization of irrigation efficiency, water availability considerations and more flexible irrigation schedules that can be tailored to represent typical field practices. Conducting parallel testing and assessment of future developments covering greater spatial and temporal scales (e.g. in the form of long-term observatories) will be crucial, especially as more accurate irrigation data becomes available.

## 4.5 Conclusions

This study assessed the ability of the CLM5-FruitTree sub-model to represent irrigation practices in fruit orchards in a small Mediterranean catchment and explored the effects of different irrigation scenarios on simulated yield and CWUE. The standard CLM5 irrigation routine could not accurately reproduce observed irrigation practices, which motivated the implementation of an irrigation data stream that directly prescribes measured irrigation data. Using this irrigation data stream, observed SM dynamics in the two studied apple orchards were well captured by the model. We did however find some discrepancies between observed and simulated SM, transpiration, and yield that were related to uncertainties in soil hydraulic parameters and limitations in the crop representation, which does, for instance, not account for the active grass cover growing in the alleys.

To examine the potential to improve regional irrigation management using CLM5, we simulated different irrigation scenarios and analyzed their effect on crop yield and CWUE. The model showed distinct effects of deficit irrigation on yield and CWUE for scenarios with 25% and 50% reduction in irrigation (DI75 and DI50, respectively) that were tested using the irrigation data stream. While DI75 had negligible negative effect on yield and CWUE, DI50 notably reduced both yield and CWUE. Based on the modelling results, this would suggest substantial water savings of up to 125 mm year<sup>-1</sup> with little to no effect on apple yields and up to 250 mm year<sup>-1</sup> when accepting up to 30% reduction in yield (although potential effects of fruit quality need to be considered as well). These effects varied depending on climatic conditions, soil type, and timing of irrigation. Hence, under limited water availability, irrigation should primarily focus on the summer months July to September and on sandy soils with lower water holding capacity.

The outcomes of this study demonstrate the potential use of CLM5 in irrigation and water resources management research and applications. Future research efforts should focus on improving soil and crop parameterizations, and as well as process representation. Finally, we anticipate that implementing more realistic irrigation schedules in land surface models such as CLM5 will allow for better water resource management at the local and regional level.





# 5 Synthesis

In the face of increasing water scarcity in the Mediterranean and other arid and semi-arid regions, tools to effectively determine crop specific irrigation requirements are crucial to sustain agricultural production and to guide irrigation and water resources management decisions. To achieve this a multifaceted approach is needed that involves:

- Affordable measurement technology that can provide comprehensive, high-resolution environmental data on climate, soil, and vegetation.
- Physically-based, fully distributed predictive models that accurately represent agricultural systems and the effect of irrigation management on yield, water resources, and other components of the terrestrial system.

In the following synthesis, the contribution this thesis has made to both of these components is summarized and promising directions for further research are discussed. Lastly, potential applications for different aspects of irrigation and water resources management at the field scale and beyond are explored.

## 5.1 Towards high-resolution climate data using low-cost sensors

High-resolution climate data is critical to improve the resilience and sustainability of the agricultural sector. This is especially important in light of more frequent and intense weather extremes related to climate change that decision-makers will be confronted with. The evaluation of a low-cost all-in-one weather station demonstrated that this type of sensor can deliver reliable and timely observations of local microclimatic conditions. As such, it is well suited for application in precision agriculture to promote water conservation, tailor management decisions to crop needs, and reduce the risk of crop failure through early warning systems. The potential of all-in-one weather stations to increase data availability and resolution in data-scarce, remote, and heterogeneous regions, and under budget constraints will benefit the quality of local and regional

modelling and a range of applications. These include water resources management [Jencso *et al.*, 2019], weather forecasting [Hewage *et al.*, 2020], early warning systems for flood prediction [Ibarreche *et al.*, 2020; Nikolić *et al.*, 2022], and urban planning [Bassett *et al.*, 2016; Šećerov *et al.*, 2019], which are of importance not only to farmers but also to policy-makers, industries, and the general population. In any case, reliability and accuracy of the deployed sensors should meet the needs of the intended purpose, as this work also revealed that data from low-cost weather stations are associated with higher uncertainties compared to that of high-end measurement devices. This can have important implications for instance regarding their use in extreme weather research. Here, current design, size, or sensor quality may not be well fit to deliver reliable measurements under strong winds, heavy rain, or solid precipitation.

## **5.2 Towards improved process-based modelling of agricultural systems**

In conjunction with environmental data, process-based models are increasingly being used for the simulation and sustainable management of agricultural systems. However, crops in such models are often not sufficiently differentiated or rather certain crop types are not considered at all [Blyth *et al.*, 2021; Lombardozzi *et al.*, 2020; Peng *et al.*, 2020]. Consequently, systems with diverse crops and agricultural practices, e.g. the Mediterranean that is largely characterized by permanent crops (e.g. fruit trees), are poorly represented. In this work, the widely used global LSM CLM5 was extended by a component that enables the consideration of apple orchards (CLM5-FruitTree). By capturing the prolonged growing season, permanent woody biomass, and typical management practices of fruit trees, CLM5-FruitTree offers new possibilities to address relevant research questions in Mediterranean agricultural catchments or other fruit growing regions. Particularly, the impacts of land use and climate change on crop production and crop water requirements in the Mediterranean can be investigated more reliably. This kind of analysis can reveal potential shifts in crop phenology and changes in water demand or suitable growing areas for fruit trees, which can have important implications for food security [Fader *et al.*, 2015]. Another topic that could be addressed with the model development is the potential of orchards to sequester C and help mitigate climate change impacts [Sharma *et al.*, 2021; Wu *et al.*, 2012]. This potential depends on

orchard age, biomass production, and management, as well as climatic conditions which could be jointly investigated with CLM5-FruitTree.

There is a number of additional model developments that can be envisaged to further improve the simulation of fruit orchards. Some of these improvements involve additional refinements of the new crop model routine. One model weakness that should be resolved is the failure to capture the inter-annual yield variability of fruit trees, as accurate yield prediction is essential for farmers as well as policy makers to maximize economic profit and reduce losses. This could potentially be addressed by adding parameterizations of alternate bearing and flowering, both of which greatly affect final yield. The resource budget model for alternate bearing, first introduced by *Isagi et al.* [1997], could present a possible approach in this direction. It assumes that flowers are only produced once C reserves exceed a certain threshold which could be integrated into the existing C reserve dynamics in CLM5-FruitTree. Another aspect of yield which is currently not accounted for is fruit quality, which plays an important role in fruit production. Coupling or integration of a dedicated fruit tree model such as QualiTree that includes the effect of management on fruit quality could be explored in this context [*Lescourret et al.*, 2011; *Miras-Avalos et al.*, 2013]. Moreover, the options for crop management could be further extended to include their effect on C and water fluxes in the orchard. For instance, mulching is widely used in semi-arid and arid environments for annual crops [*Chakraborty et al.*, 2008] as well as fruit orchards [*Liao et al.*, 2021; *Liu et al.*, 2014]. In CLM5-FruitTree, the effect of mulching was only crudely considered by adding more C to the soil in the form of pruned biomass but did not include its effect on soil water retention and evaporation. To account for this, two recent studies could be explored that have incorporated a (plastic) mulch layer into a surface energy balance model and a LSM, which allowed to examine its effect on surface energy fluxes and ET [*Ochege et al.*, 2022; *Yuan et al.*, 2019].

Certain other model improvements necessitate more substantial changes to the model structure or physics but could significantly advance the representation of the true land-surface heterogeneity and pave the way towards the modelling of more complex vegetation structures. One of these improvements concerns the partitioning of energy and the transfer of heat and water within different canopy structures. The current assumption of a closed canopy, typical for annual crops, needs to be revisited to reduce uncertainties in the simulation of energy balance and water cycle in fruit orchards or other

heterogeneous canopies. Under water-limited conditions this is especially important to accurately determine crop water requirements [Gao *et al.*, 2020; Ma and Liu, 2019]. A possible way forward may be the explicit modelling of different surfaces as proposed by Blyth *et al.* [2021] or an advanced multi-layer canopy model to improve sub-canopy processes as tested by Ma and Liu [2019]. Another major topic involves the types of planting systems that can be represented in CLM5. Currently, only homogenous annual cropping systems are modelled that differ significantly from orchard systems where tree rows alternate with alleys, which are often covered by weeds or cover crops. Implementing such intercropping or mixed cropping systems in CLM5 would improve the simulation of C and water fluxes and could furthermore create opportunities to extend the model towards the simulation of agro-forestry and other diversified cropping systems. Such systems could regain more relevance as they can support soil water retention, C sequestration, biodiversity, and food security [De Stefano and Jacobson, 2018; Debaeke *et al.*, 2017]. In their review, Hernández-Ochoa *et al.* [2022] identified several agro-ecosystem models that can represent such systems to a certain extent and which could serve as a basis for this kind of development in CLM5.

Any process-based model used to simulate the Mediterranean agricultural system needs to consider irrigation as a critical management practice to meet crop water requirements. While the land modelling community has recognized irrigation as an important driver of change in the water cycle and other processes occurring at the land surface, it is still not accurately accounted for in most LSMs. Therefore, the final part of this work focused on assessing and improving the representation of irrigation in the context of field-scale and regional irrigation management in fruit orchards using CLM5-FruitTree. Local weather data and parallel observation of SM and irrigation at the field scale were essential to quantify the model performance after making site-specific adjustments to soil, crop, and irrigation parameterizations. The models' ability to approximate observed irrigation quantities depended on how well root zone SM and water movement was simulated throughout the soil profile. Furthermore, it became evident that additional flexibility in the irrigation routine is necessary to represent farmers' irrigation practices. A confident validation of the total crop water requirements proved more challenging as only a part of ET was observed using sapflow measurements that were additionally associated with a large measurement uncertainty. At catchment scale, the explorative analysis of different irrigation scenarios gave interesting insights into expected yield and CWUE under

varying irrigation amounts, and the additional role of soil and climate in driving the magnitude of the effect of reduced irrigation. Overall, this analysis showed that CLM5 could produce relevant information to advice farmers, water authorities, and policy makers in irrigation management at different scales. Additional simulations with projections of future climate conditions can furthermore shed light on how water consumption will likely develop. Together with a more flexible irrigation routine that considers different irrigation techniques and strategies, irrigation management could be optimized to ensure high yields while minimizing water consumption.

Towards the use of CLM5 for these applications, uncertainties that are related to model processes and parameterizations need to be addressed. This is critical to ensure crop water requirements and irrigation amounts can be predicted accurately. For instance, there is large uncertainty associated with the parameters used to describe plant hydraulic stress (PHS routine) which are currently generic for all crops in CLM5. An initial assessment of the current parameterization suggested a generally low sensitivity of crops to water stress. It is, however, well established that different crops and crop varieties react differently to water stress and levels of SM depletion [Budak *et al.*, 2013; Chaves *et al.*, 2003]. Consequently, the model may not accurately represent stressed conditions for a particular crop, which limits its ability to determine optimal irrigation amounts or assess the trade-off between yield loss and water savings under various deficit irrigation scenarios. This also adds ambiguity to the calibration of the SM threshold parameter to trigger irrigation, as crop- and growth stage specific differences regarding the optimal threshold are most likely not well captured. Enhancing calibration efforts for these parameters will therefore be critical. Furthermore, some authors have suggested the implementation of more advanced approaches to better represent plant stress for different plant types. Verhoef and Egea [2014] suggested to combine plant and soil hydraulics with chemical signalling instead of a water stress factor that is calculated based on SMP, as it is currently used in CLM5. Another approach may be to additionally incorporate leaf water potential for an improved plant stress representation [Kennedy *et al.*, 2019]. Another issue, which was not yet discussed in this work is the simplified root profile representation in LSMs, which was found to introduce considerable uncertainty in root water uptake simulations [Canal *et al.*, 2014; Zeng, 2001]. For example, Zeng [2001] showed that the one-parameter equation used for the rooting profile in CLM5 resulted in a too shallow rooting profile, which could explain some of the observed SM biases in the

deeper soil layers. Addressing such model uncertainties will be relevant when evaluating deficit irrigation strategies or the need for irrigation in fields that are partially or entirely rainfed. In fact, under such conditions, crops can develop extensive root systems to tap deep soil water or shallow groundwater, particularly perennial crops [Vico and Brunsell, 2018]. Different approaches using a two-parameter equation [Zeng, 2001] or uniform instead of exponential root profiles [Stevens *et al.*, 2020] have been suggested next to upscaling a 3D hydraulic root architecture model [Vanderborght *et al.*, 2021], and should be further explored to improve root profile representation in CLM5.

Future model developments to improve the representation of agricultural systems and irrigation in LSMs such as CLM5 are driven by a diverse user community including crop modellers, hydrologists, climate scientists, ecologists, and many others. Such community-based model development greatly benefits from a multidisciplinary knowledge base but also faces challenges to integrate the various spatiotemporal scales that are targeted by different groups of researchers [Blyth *et al.*, 2021; Peng *et al.*, 2020]. Another difficulty comes with finding parameters for the static global parameterization that is used for crop and irrigation parameters in CLM5, as developments are often made for a specific region and dataset, and cannot be easily adapted to the global scale. The development of CLM5-FruitTree is no exception to this, as despite the comprehensive dataset, the geographic scope and timeframe were limited considering only a few seasons and a single location. Lombardozzi *et al.* [2020] therefore proposed that future model developments should focus on moving to spatially varying parameterizations instead of global parameters to better represent regional differences and crop adaptations to their environment. The crop calendar developed by Rabin *et al.* [2023] or the implementation of spatially explicit irrigation parameters could improve the models accuracy and/or flexibility to capture such differences in crop growing season and irrigation management, respectively. Either way, there is a great need for spatially continuous data concerning soils, crops, irrigation amounts, or water withdrawal for model calibration and validation across different scales [Blyth *et al.*, 2021; Gibson *et al.*, 2017; Pongratz *et al.*, 2018]. At the same time, the data should be available at a sufficient resolution (i.e. < 1 km) to produce results that are relevant for individual farmers and local authorities. Therefore, efforts to obtain the necessary data need to be continued and intensified. These may include the combined use of high-resolution satellite datasets and machine learning algorithms to retrieve irrigation extent and amount [Dari *et al.*, 2022; Zappa *et al.*, 2021],

land cover [Li *et al.*, 2022], crop phenology [Gao and Zhang, 2021], or yield estimates [Hunt *et al.*, 2019]. Moreover, long-term in-situ observations from new shared research infrastructures such as eLTER [Mirtl, 2018] and ICOS [Heiskanen *et al.*, 2022] as well as existing environmental observatories (see Section 1.1.4) are valuable sources of distributed data (e.g., atmospheric, ecosystem, biological, soil parameters). Finally, the expansion of non-traditional data sources from the rapidly developing smart farming and citizen science movements, and private sensor networks may be used for model input, calibration, and validation at improved spatiotemporal resolution in the future [Fraisl *et al.*, 2022; Reis *et al.*, 2015; Tsai *et al.*, 2021].

Such joint efforts in model development and calibration could enable the application of LSMs such as CLM5 for different aspects of irrigation and water resources management across a range of spatiotemporal scales. In the following, some possible applications in this context are explored that build on the potential of LSMs such as CLM5 as tools for research and decision-making.

### 5.3 Operational field-scale irrigation scheduling using CLM5

Effective irrigation scheduling is one potential way to minimize water wastage while ensuring optimal yield for the farmer. Further developing the existing model application at field scale into an operational tool for irrigation scheduling in a smart farming context could therefore be a promising extension of this work. Because irrigation in CLM5 is based on SM, determining the optimal irrigation amount necessitates, above all, an accurate representation of SM conditions.

To improve field-scale SM simulations a data assimilation framework could be applied in fields where SM is being monitored continuously. Data assimilation of SM can improve model simulations through the update of the models' SM state and the optimization of relevant model parameters, in this case, soil hydraulic parameters [Reichle *et al.*, 2007; Strebel *et al.*, 2022]. In addition, estimates of uncertainty in SM can be obtained that can be used to quantify the uncertainty in, e.g. the prediction of irrigation requirements or yield outcome [De Lannoy *et al.*, 2019]. Assimilation of SM into various LSMs has been performed previously to improve SM predictions for cropland and natural vegetation [Hung *et al.*, 2022; Kolassa *et al.*, 2017; Mahmood *et al.*, 2019; Naz *et al.*, 2019]. Han *et*

*al.* [2016] and *Li et al.* [2018] presented first studies using data assimilation for irrigation scheduling in drip irrigated citrus orchards in CLM4.5 with promising results and the possibility of real-time online control for the latter study. For CLM5, *Strebel et al.* [2022] recently performed and tested the coupling to PDAF (the parallel data assimilation framework) which could be applied to continue the present work and to test if the bias in simulated SM can be reduced.

The improved model simulations can further be combined with suitable short- to medium-range weather forecasts [*Hewage et al.*, 2020; *Lorite et al.*, 2015] to predict the depletion of SM within the forecasting window. Subsequently, the optimal irrigation amount and timing can be determined based on a defined target SM or SMP to avoid crop water stress while minimizing water wastage. By using ensemble weather forecasts or historical weather data as forecasts, uncertainties in the predictions could be taken into account [*Guo et al.*, 2023; *Linker and Sylaios*, 2016]. Additionally, alternative decisions of irrigation timing could be considered and the trade-off and risks between water consumption and crop stress could be communicated to the farmer to support decision-making [*Guo et al.*, 2023]. Automating the entire process, including the fetching and preparation of data for model input, starting a new model run, analysing model output, and communicating the proposed irrigation schedule to the farmer, entails the development of a web application and the necessary APIs (application programming interfaces) that allow communication between the different software applications and data portals. This is not trivial, as setting up and running CLM5 and similar models involves a multi-step process that requires a significant amount of expert knowledge and computational resources. Developing a simplified modelling infrastructure by, e.g., unifying workflows, creating templates, or building simple user interfaces can support operational use of the model. Moreover, major efforts must also be made to improve interoperability between different applications as well as for the harmonization and shared use of data [*Choi et al.*, 2021; *Maechling et al.*, 2005].

Application of the described irrigation scheduling service in combination with data assimilation necessitates the availability of continuous SM data that is representative for the target area. At present, WSNs may be the most effective solution for small, heterogeneous fields. The number of sensors and thus total costs associated with the installation of such a network will depend on several factors including the heterogeneity of soil texture, crop planting patterns, and management practices. Electromagnetic or



drone-based soil and crop surveys can be used to decide on an optimal sensor placement [Hedley *et al.*, 2012; von Hebel *et al.*, 2021]. Alternatively, non-invasive measurement techniques such as cosmic ray neutron sensing that provide an integrated SM measurement over multiple hectares could be used as the technique becomes more cost-effective. This way multiple growers could invest into a few shared sensors to lower investments for the individual and to share the benefit of improved SM simulations.

While the costs of sensing technologies are steadily decreasing, many farmers, especially in the low to middle-income countries of the Mediterranean region, lack financial assets and technical knowledge to install and maintain such extensive measurement systems. The complexity of model-based irrigation scheduling and scepticism or low confidence in this technology result in low adoption rates especially for small-scale irrigators [Barnes *et al.*, 2019; Fernández García *et al.*, 2020; Frisvold and Deva, 2012]. It is therefore critical that governments and water authorities support sustainable irrigation management at the farm scale through funding and training, or educational programmes based on regional and national water management plans that consider irrigation in the larger context of water resources.

## **5.4 Modelling frameworks for holistic irrigation and water resources management**

So far, this work has considered field and regional scale irrigation under the assumption of an unrestricted supply of suitable irrigation water or hypothetical scenarios of limited water availability (deficit irrigation scenarios). It is however clear, that this does not reflect reality in the Mediterranean context, where instead, irrigation is restricted by water availability and quality, and competes with other water use sectors (e.g., agricultural, urban, industrial, environmental) [Choukr-Allah *et al.*, 2012]. Modelling for regional water resources management needs to consider this interconnectedness to ensure the responsible use and long-term sustainability of groundwater and surface water resources across sectors.

Groundwater is the main water resource in most semi-arid and arid Mediterranean catchments including the PHO [Pisinaras *et al.*, 2018; Zagana *et al.*, 2007] but also the more water rich Adige valley [Castagna *et al.*, 2015]. Taking water availability for

irrigation into account should therefore consider groundwater and the impact of irrigation activities on groundwater dynamics (depletion or recharge) in the catchment. The work of *Felfelani et al.* [2021] could be a good starting point, as they implemented a prognostic groundwater module into CLM5 that considers aquifer pumping as well as intercell lateral flow. This improved groundwater level simulations as well as the subsurface response to pumping. Apart from representing the impact of groundwater withdrawals on the surrounding areas, the implementation of intercell lateral flow will likely also improve the representation of aquifer recharge mechanisms. In the PHO but also in other Mediterranean catchments with a pronounced topographic gradient, precipitation and snow melt from the mountainous parts of the catchment contribute substantially to aquifer recharge while the lowland typically contributes little to total annual recharge [*Pisinaras et al.*, 2018; *Zagana et al.*, 2007]. Alternatively, a better representation of subsurface hydrological processes and interactions with the land surface can be achieved by coupling CLM5 with more complex hydrological models such as ParFlow or groundwater models such as MODFLOW [*Felfelani et al.*, 2022]. In this way, groundwater resources can be better assessed, and a sustainable level of water abstraction can be determined more reliably. Moreover, effective mitigation measures to avoid the overexploitation of groundwater aquifers, such as deficit irrigation strategies or the switch to less water consuming or more drought resilient crops, can be explored. *Peng et al.* [2020] argued that to reliably investigate such adaptation and mitigation strategies a much greater effort to merge agro-economic CMs and LSMs is necessary. In this way the strength of CMs in representing the effect of environmental conditions and crop management on yield can be combined with the ability of LSMs to jointly consider agricultural systems and other land uses as well as their environmental implications on other Earth system components such as C and water cycles.

In moving towards integrated water resources management, models used as decision-making tools must reflect the multi-purpose function of water resources and the multidisciplinary nature of their management. This entails the consideration of other water use sectors including industrial, recreational, domestic, and environmental as well as artificial water reservoirs used for irrigation or other purposes [*Felfelani et al.*, 2021]. Furthermore, future model developments may also consider alternative water sources from wastewater recycling or desalination plants, since they will likely grow in importance as water scarcity in Mediterranean countries continues to worsen [*Ait-Mouheb*

*et al.*, 2020; *Martin-Gorriiz et al.*, 2014; *Martínez-Alvarez et al.*, 2019; *Moretti et al.*, 2019]. The use of such water sources comes with increased energy consumption, environmental impacts, and economic costs on top of possible health concerns that undermine their social acceptance [*Ait-Mouheb et al.*, 2020; *Martínez-Alvarez et al.*, 2019]. Therefore, the combination of environmental, economic, and social goals in the integrated approach to water resources management could be combined with the water-energy-food nexus concept to achieve higher resource efficiency and increased water, energy, and food security [*Shams and Muhammad*, 2022]. In this context a stronger integration or exchange of information between LSMs (or fully coupled Earth System Models) with models from other communities such as integrated assessment, vulnerability, and adaptation should be encouraged to create holistic modelling frameworks for water resources management [*Van Vuuren et al.*, 2012].



# Appendix

## Appendix I Full time series ATMOS41

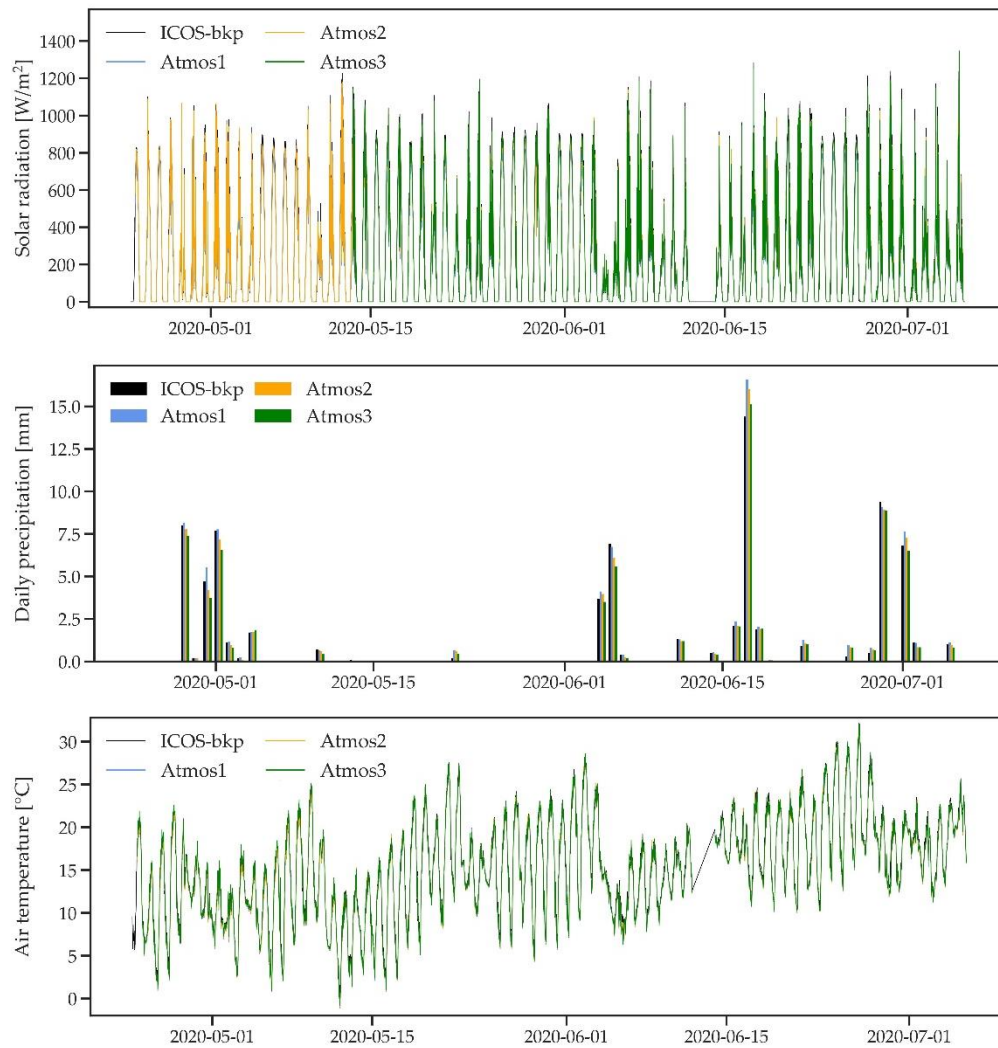


Figure A.1 *Cont.*

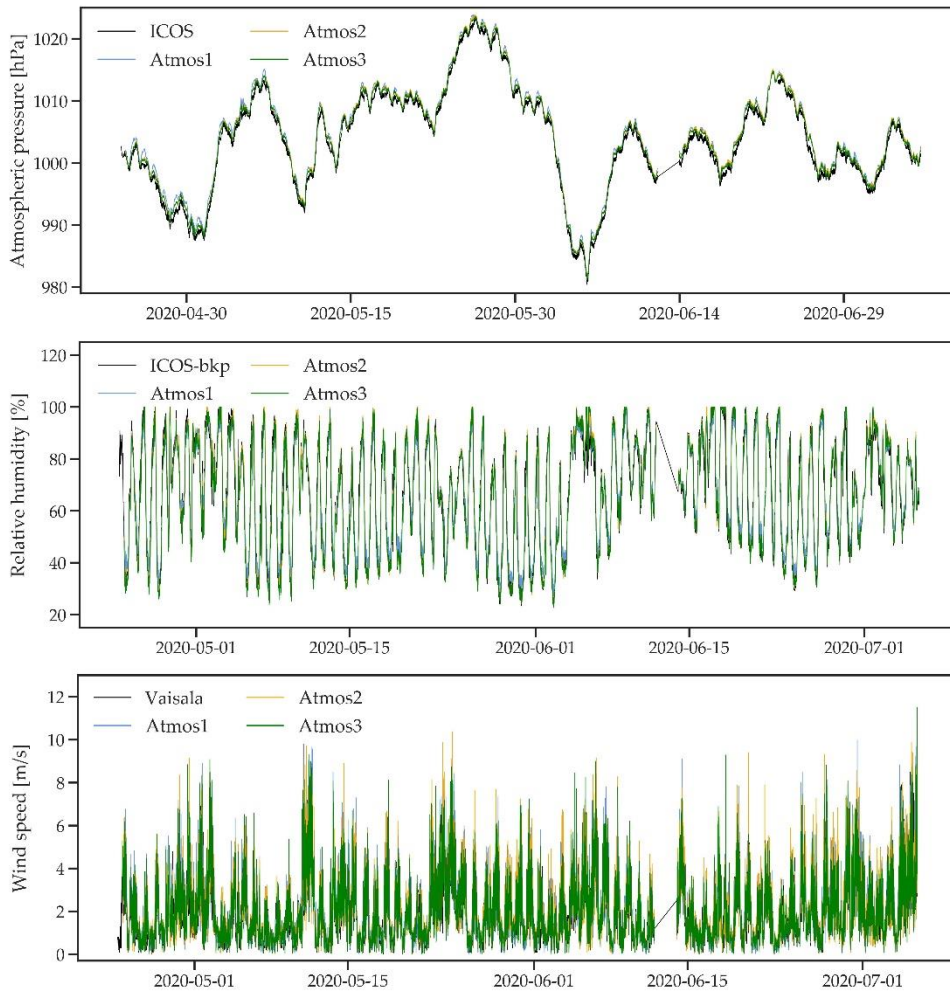


Figure A.1 Full time series for all standard weather variables measured by three ATMOS41 weather stations and the reference station.

## Appendix II Linear regression ATMOS41

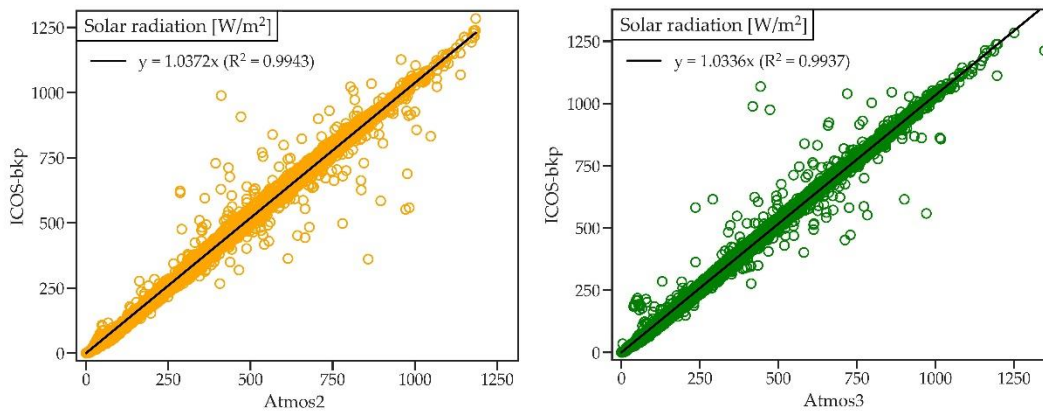


Figure A.2 Linear regression for solar radiation for Atmos2 and Atmos3 vs. ICOS-bkp station.

### Appendix III Sequential model for bud break prediction

The bud break prediction in CLM5-FruitTree is based on the sequential model developed by *Cesaraccio et al.* [2004]. Negative chill days ( $C_d$ ) are accumulated from the 1<sup>st</sup> of November followed by positive anti-chill days ( $C_a$ ) to overcome the different stages of tree dormancy, rest and quiescence. The chilling requirement ( $C_R$ ) defines the threshold for the accumulation of  $C_d$  and is reached when  $\sum C_d \leq C_R$ . Thereafter  $C_a$  accumulation begins until  $C_R + \sum C_a \geq 0$  at which bud break occurs. The accumulation of  $C_d$  and  $C_a$  on a given day is calculated from maximum ( $T_x$ ) and minimum ( $T_n$ ) daily air temperature as well as a temperature threshold for chill accumulation ( $T_C$ ), and varies depending on five possible temperature cases that relate  $T_x$ ,  $T_n$ ,  $T_C$ , and  $0^\circ\text{C}$  with the daily mean air temperature (Table A.1). The optimal values for  $C_R$  and  $T_C$  were calibrated based on bud break observations from 2010–2013 for the Adige site by minimizing the RMSE between observations and predicted bud break. The optimal value for  $C_R$  was -68 while  $T_C$  was  $4^\circ\text{C}$  resulting in an RMSE of 7.2 days.

Table A.1 Chill day ( $C_d$ ) and anti-chill day ( $C_a$ ) calculation for five different temperature cases relating maximum ( $T_x$ ) and minimum ( $T_n$ ) air temperature to the air temperature threshold ( $T_C$ ) and  $0^\circ\text{C}$ ,  $T_M$  is the air mean temperature.

| Temperature Cases              | Chill days  | Anti-chill days                            |
|--------------------------------|---|--|
| $0 \leq T_C \leq T_n \leq T_x$ | $C_d = 0$   | $C_a = T_M - T_C$                          |
| $0 \leq T_n \leq T_C < T_x$    | $C_d = - \left[ (T_M - T_n) - \frac{(T_x - T_C)^2}{2(T_x - T_n)} \right]$ | $C_a = \frac{(T_x - T_C)^2}{2(T_x - T_n)}$ |
| $0 \leq T_n \leq T_x \leq T_C$ | $C_d = -(T_M - T_n)$  | $C_a = 0$                                  |
| $T_n < 0 \leq T_x \leq T_C$    | $C_d = - \left[ \frac{T_x^2}{2(T_x - T_n)} \right]$                       | $C_a = 0$                                  |
| $T_n < 0 < T_C < T_x$          | $C_d = - \frac{T_x^2}{2(T_x - T_n)} - \frac{(T_x - T_C)^2}{2(T_x - T_n)}$ | $C_a = \frac{(T_x - T_C)^2}{2(T_x - T_n)}$ |

## Appendix IV Calculation of incoming longwave radiation

Incoming longwave radiation ( $LW_{in}$ ) can be expressed based on the Stefan Boltzmann Law as:

$$LW_{in} = \varepsilon_{eff} * \sigma * T^4 = \varepsilon_{cs} * F * \sigma * T^4 , \quad (A.1)$$

where  $\varepsilon_{eff}$  is the effective emissivity that can be expressed by multiplying the clear-sky atmospheric emissivity  $\varepsilon_{cs}$  with a cloud factor  $F$  (always  $\geq 1$ ) that expresses the increase of  $LW_{in}$  under cloudy conditions,  $\sigma$  is the Stefan Boltzmann constant ( $5.67 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-1}$ ) and  $T$  is the 2m air temperature in K.

Clear-sky emissivity was obtained using the *Konzelmann et al.* [1994] parameterization as follows:

$$\varepsilon_{cs} = 0.23 + 0.484 * \left(\frac{e}{T}\right)^{\frac{1}{8}} , \quad (A.2)$$

where  $e$  is the vapour pressure in Pa at 2 m.

Equation (A.1) can be rearranged to obtain  $F$  as follows:

$$F = \frac{LW_{in}}{\varepsilon_{cs} * \sigma * T^4} \quad (A.3)$$

$F$  was calculated at hourly interval using measured  $LW_{in}$  data from 2010 and  $\varepsilon_{cs}$  calculated using the above Eq. (A.2).

As proposed by *Sedlar and Hock* [2009], in the absence of cloud data, the cloud factor  $F$  can be parameterized as a function of the atmospheric transmissivity index  $\tau$ , which is defined as follows:

$$\tau = \frac{SW_{in}}{SW_{toa}} , \quad (A.4)$$

where  $SW_{in}$  is the incoming shortwave radiation, and  $SW_{toa}$  is the theoretical shortwave radiation received at the top of the atmosphere.

Figure A.3 shows the linear equation that was fitted to the relationship of  $F$  and  $\tau$  for the year 2010. For the calculation of clear-sky emissivity, all data where  $\tau$  was greater than 0.7 (N=3863) was considered based on the suggestion by *Campbell* [1985].



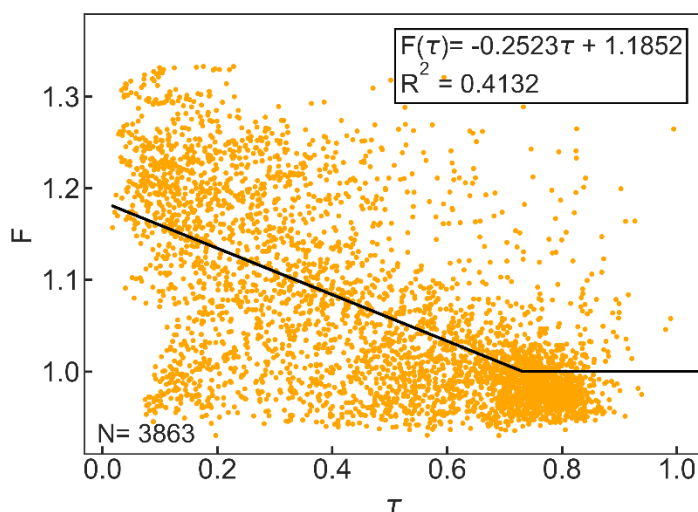


Figure A.3 Cloud factor  $F$  as a function of atmospheric emissivity  $\tau$  for hourly observations. The black line represents the linear equation for  $F(\tau)$  and  $F \geq 1$ . Clear-sky emissivity is parameterized based on *Konzelmann et al.* [1994].

For the nighttime values and for very low incoming shortwave radiation ( $SW_{in} < 15 \text{ W m}^{-2}$ ),  $\tau$  was gap-filled with the mean of the two surrounding values to obtain a complete time series of  $LW_{in}$  data. Figure A.4 shows the results of the  $LW_{in}$  parameterization compared to  $LW_{in}$  calculated by CLM5 and to the observed data for the year 2010. As performance statistics the Pearson coefficient of correlation ( $r$ ), the root mean square error (RMSE) and percent bias (%bias) are given.

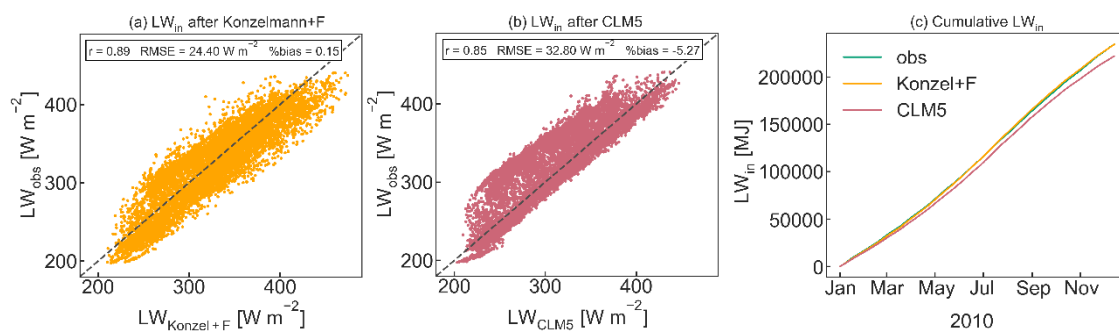


Figure A.4 Comparison of observed  $LW_{in}$  with the parameterization using (a) *Konzelmann et al.* [1994] according to Eq. (A.2) and the cloud factor parameterization  $F(\tau)$ , and (b) the calculation procedure used in CLM5, as well as (c) cumulative observed and calculated  $LW_{in}$  for 2010. Pearson's  $r$ , RMSE and %bias are given as performance statistics.



## Appendix V Parameters used in CLM5-FruitTree and for the apple PFT

Table A.2 Parameters adapted or added in the new CLM5-FruitTree sub-model and the apple PFT including phenology, CN allocation, photosynthesis, vegetation structure as well as optical and respiration parameters. Parameters were adjusted based on field observations or literature values and are listed with their definition, unit, value, and references to the literature.

| Parameter                      | Definition  | Unit        | Value  | Reference   |
|--------------------------------|---|-------------|--------|---|
| <b>Phenological parameters</b> |   |             |        |   |
| baset                          | Base temperature for GDD accumulation                                 | °C          | 4      | Based on commonly used values for apple trees [Díez-Palet <i>et al.</i> , 2019; Penzel <i>et al.</i> , 2020; Reyes <i>et al.</i> , 2016]                            |
| crequ                          | Chilling requirements for bud break of fruit tree crops               | unitless    | -68    | Calibrated using bud break dates from Zanutelli <i>et al.</i> [2013] and Zanutelli <i>et al.</i> [2015], and the sequential model [Cesaraccio <i>et al.</i> , 2004] |
| crit_temp                      | Critical temperature to initiate leaf senescence for fruit tree crops | K           | 278.15 | Adjusted based on LAI measurements [Zanutelli <i>et al.</i> , 2013]   |
| grnfill* (GDDfruit)            | GDD needed from bud break to beginning of fruit development           | degree days | 400    | Based on observed and commonly used values for apple trees [Lakso <i>et al.</i> , 2000; Neumann, 2020; Penzel <i>et al.</i> , 2020; Zanutelli <i>et al.</i> , 2013] |
| grnrp*(GDDripe)                | GDD needed from bud break to the fruit ripening phase                 | degree days | 1100   | Based on observed and commonly used values for apple trees [Lakso <i>et al.</i> , 2000; Neumann, 2020; Penzel <i>et al.</i> , 2020; Zanutelli <i>et al.</i> , 2013] |
| huileaf (GDDleaf)              | GDD accumulated at the moment of bud break (end of dormancy period)   | degree days | –      | Calculated based on sequential model for bud break prediction [Cesaraccio <i>et al.</i> , 2004]   |
| hybgdd* (GDDmat)               | GDD needed from bud break until fruit harvest                         | degree days | 2880   | Based on observed and commonly used values for apple trees [Lakso <i>et al.</i> , 2000; Neumann, 2020; Penzel <i>et al.</i> , 2020; Zanutelli <i>et al.</i> , 2013] |

## APPENDIX

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|                      |   |                                |       |  |
|----------------------|---|--------------------------------|-------|--|
| laimx*               | Maximum leaf area index                                     | m <sup>2</sup> /m <sup>2</sup> | 3     | Based on observed and commonly used values for apple trees [ <i>Li et al.</i> , 2002; <i>Valancogne et al.</i> , 1999; <i>Zanotelli et al.</i> , 2013]                       |
| lformat*(GDDlformat) | GDD needed from bud break to canopy maturity                | degree days                    | 1350  | Based on observed and commonly used values for apple trees [ <i>Lakso et al.</i> , 2000; <i>Neumann</i> , 2020; <i>Penzel et al.</i> , 2020; <i>Zanotelli et al.</i> , 2013] |
| max_NH_harvest_date  | maximum harvest date for northern hemisphere (NH)           | date (md)                      | 1015  | Based on typical harvest dates in NH   |
| max_NH_planting_date | maximum planting date for NH                                | date (md)                      | 101   | Only needed for orchard establishment and initiation of sequential model for bud break, tree is still dormant  |
| min_NH_planting_date | minimum planting date for NH                                | date (md)                      | 101   | Only needed for orchard establishment and initiation of sequential model for bud break, tree is still dormant  |
| mxmat                | Maximum orchard age   | days                           | 9125  | Based on common values for apple orchards [ <i>Lakso et al.</i> , 2000; <i>Penzel et al.</i> , 2020; <i>Zanotelli et al.</i> , 2013]   |
| ndays_stor           | Length of period for storage growth of fruit tree crops     | days                           | 50    | Based on common values for fruit orchards [ <i>DeJong and Grossman</i> , 1994; <i>Kozlowski</i> , 1992; <i>Wünsche and Lakso</i> , 2000]                                     |
| perennial            | Binary flag for perennial crop phenology                    | unitless                       | 1     |  |
| root_dmx             | Maximum rooting depth of crops                              | m                              | 0.8   | Based on observed rooting depth [ <i>Zanotelli et al.</i> , 2013]  |
| rootprof_beta*       | Rooting beta parameter, for C and N vertical discretization | unitless                       | 0.964 | Calibrated based on root sampling campaign of root mass up to 60cm ( <i>Zanotelli</i> 2010, unpublished data)  |
| woody                | Binary flag for woody lifeform                              | unitless                       | 1     |  |

**C and N allocation parameters**

|            |  |          |      |   |
|------------|--|----------|------|---|
| aleaff*    | Final leaf allocation coefficient  | unitless | 0.01 | Adjusted based on monthly biomass measurements [Zanotelli <i>et al.</i> , 2013] |
| aleafstor* | Leaf allocation coefficient to storage post-harvest used in CNAllocation | unitless | 0.3  | Adjusted based on monthly biomass measurements [Zanotelli <i>et al.</i> , 2013] |
| allconss*  | Power to control the shape of the stem allocation curve                  | unitless | 1.5  | Adjusted based on monthly biomass measurements [Zanotelli <i>et al.</i> , 2013] |
| arootf*    | Root allocation coefficient at start of fruit development                | unitless | 0.2  | Adjusted based on monthly biomass measurements [Zanotelli <i>et al.</i> , 2013] |
| arootf2*   | Final root allocation coefficient until harvest                          | unitless | 0.08 | Adjusted based on monthly biomass measurements [Zanotelli <i>et al.</i> , 2013] |
| arooti*    | Initial root allocation coefficient                                      | unitless | 0.7  | Adjusted based on monthly biomass measurements [Zanotelli <i>et al.</i> , 2013] |
| astemf*    | Final stem allocation coefficient]                                       | unitless | 0.22 | Adjusted based on monthly biomass measurements [Zanotelli <i>et al.</i> , 2013] |
| bfact*     | Exponential factor used for fraction allocated to leaf                   | unitless | -0.5 | Adjusted based on monthly biomass measurements [Zanotelli <i>et al.</i> , 2013] |
| declfact*  | Decline factor to control the shape of the stem allocation curve         | unitless | 4    | Adjusted based on monthly biomass measurements [Zanotelli <i>et al.</i> , 2013] |
| fcur*      | Fraction of C and N allocated to the displayed pools                     | unitless | 0.95 | Tuned based on observed LAI and yield data [Zanotelli <i>et al.</i> , 2013]     |
| fleafi*    | Initial leaf allocation coefficient                                      | unitless | 0.85 | Adjusted based on monthly biomass measurements [Zanotelli <i>et al.</i> , 2013] |
| flivewd    | Fraction of new wood that is live  |          | 0.15 | Same as BDT in CLM5   |

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|            |  |       |      |  |
|------------|--|-------|------|--|
| frootCN    | Fine root C:N ratio                                | gC/gN | 32   | Average of 6 measurements (Zanotelli 2010, unpublished data) |
| grainCN*   | Fruit C:N ratio                                    | gC/gN | 139  | Average of 6 measurements (Zanotelli 2010, unpublished data) |
| leafCN*    | Leaf C:N ratio                                     | gC/gN | 19.7 | Average of 6 measurements (Zanotelli 2010, unpublished data) |
| lflitCN    | Litter C:N ratio                                   | gC/gN | 60   | Average of 4 measurements (Zanotelli 2010, unpublished data) |
| livewdCN   | Livewood C:N ratio                                 | gC/gN | 60   | Average of 6 measurements (Zanotelli 2010, unpublished data) |
| transplant | Initial carbon for crops transplanted from nursery | gC    | 5    |  |

### Photosynthetic parameters

|              |  |  |       |   |
|--------------|--|--|-------|---|
| i_vcad*      | Intercept of the relationship between leaf N per unit area and $V_{cmax25top}$ | $\mu\text{molCO}_2/\text{m}^2/\text{s}$      | 5.2   | Adjusted in between BDT and crop  |
| medlynslope* | Medlyn slope of conductance–photosynthesis relationship                        | $\mu\text{molH}_2\text{O}/\mu\text{molCO}_2$ | 8.2   | Tuned based observed GPP and ET data [Zanotelli <i>et al.</i> , 2015]   |
| s_vcad*      | Slope of the relationship between leaf N per unit area and $V_{cmax25top}$     | $\mu\text{molCO}_2/\text{s}/\text{gN}$       | 34    | Tuned based on observed LAI and yield data [Zanotelli <i>et al.</i> , 2013]                                   |
| slatop*      | Specific leaf area at top of canopy  | $\text{m}^2/\text{gC}$                       | 0.028 | Mean value for the growing season based on LAI and leaf biomass measurements [Zanotelli <i>et al.</i> , 2013] |

### Vegetation structure and management

|         |   |          |      |                     |
|---------|---|----------|------|---------------------|
| displar | Ratio of displacement height to canopy top height | unitless | 0.67 | Same as BDT in CLM5 |
|---------|---|----------|------|---------------------|

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|               |  |                  |      |  |
|---------------|--|------------------|------|--|
| mulch_pruning | Binary flag for mulching (1) or export (0) of pruning material | unitless         | 1    | Based on reported organic farming practices [Zanotelli <i>et al.</i> , 2013]   |
| prune_fr      | Fraction of dead stem that is pruned                           | unitless         | 0.85 | Based on reported pruning quantity [Zanotelli <i>et al.</i> , 2015]  |
| nstem         | Planting density   | #/m <sup>2</sup> | 0.33 | Based on reported planting density [Zanotelli <i>et al.</i> , 2013]  |
| taper         | Ratio of stem height to radius at breast height                |                  | 120  | Based on reported tree allometry and height [Zanotelli <i>et al.</i> , 2013]   |
| xl*           | Leaf/stem orientation index                                    | unitless         | 0.25 | Same as BDT in CLM5  |
| z0mr*         | Ratio of momentum roughness length to canopy top height        | unitless         | 0.06 | Based on average values reported for apple [la Fuente-Sáiz <i>et al.</i> , 2017] and citrus [Tanny and Cohen, 2003] orchards |
| ztopmx        | Maximum canopy height for crops                                | m                | 3.6  | Based on reported tree heights [Zanotelli <i>et al.</i> , 2013]  |

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**Optical parameters**

|          |                             |          |      |   |
|----------|-----------------------------|----------|------|---|
| rhoInir* | Leaf reflectance: near-IR   | fraction | 0.5  | Based on average values for apple trees [Bastías and Corelli-Grappadelli, 2012] |
| rhoIvis* | Leaf reflectance: visible   | fraction | 0.1  | Based on average values for apple trees [Bastías and Corelli-Grappadelli, 2012] |
| rhoSnir* | Stem reflectance: near-IR   | fraction | 0.39 | Same as BDT in CLM5   |
| rhoSvis* | Stem reflectance: visible   | fraction | 0.16 | Same as BDT in CLM5   |
| tauInir* | Leaf transmittance: near-IR | fraction | 0.3  | Based on average values for apple trees [Bastías and Corelli-Grappadelli, 2012] |

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|          |                             |          |       |  |
|----------|-----------------------------|----------|-------|--|
| taulvis* | Leaf transmittance: visible | fraction | 0.04  | Based on average values for apple trees [ <i>Bastías and Corelli-Grappadelli, 2012</i> ] |
| tausnir* | Stem transmittance: near-IR | fraction | 0.001 | Same as BDT in CLM5  |
| tausvis* | Stem transmittance: visible | fraction | 0.001 | Same as BDT in CLM5  |

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### Respiration

|                     |   |   |       |                     |
|---------------------|---|---|-------|---------------------|
| FUN_fracfixers*     | The maximum fraction of assimilated carbon that can be used to pay for N fixation         | fraction                                | 0.25  | Same as BDT in CLM5 |
| lmr_intercept_atkin | Intercept in the calculation of the top of canopy leaf maintenance respiration base rate. | $\mu\text{molCO}_2/\text{m}^2/\text{s}$ | 1.756 | Same as BDT in CLM5 |

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