

**Strengthening process-based modelling of cropland
flux dynamics under various abiotic conditions:
Integrated assessment and development of Daisy
soil–plant–atmosphere model for a Walloon cropland**

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Abstract

Croplands play a central role in the global carbon, nitrogen and water cycles while being among the most vulnerable ecosystems to climate change and extreme weather events. Process-based models offer a valuable tool for understanding crop flux dynamics under such conditions, but require careful parameterisation. In this thesis, we therefore developed a complete modelling workflow (i.e., sensitivity analysis, calibration and validation) and made amendments to the Daisy soil-plant-atmosphere model when applied to winter wheat crops.

The global sensitivity analysis was carried out on the temporal evolution of net ecosystem exchange (NEE), latent heat (LE), sensible heat (H) and N_2O fluxes. Parameter sensitivities were found to undergo marked transitions associated with phenological stages and prevailing environmental conditions. Photosynthetic and stomatal parameters were predominant during crop growth, while deep soil hydraulic parameters were as influential during wet years, with consequences propagating throughout the entire growing season and highlighting the need for targeted field measurements at poorly-drained sites.

Daisy was subsequently calibrated against dry matter (DM), NEE, and LE simultaneously using a multi-objective optimisation algorithm and then validated. This analysis revealed a persistent trade-off between DM and NEE, likely attributable to an underestimation of heterotrophic respiration, parameterisation issues in crop carbon partitioning or systematic biases in eddy covariance measurements. An equifinality concern for LE was also identified, probably arising from the structural decoupling of soil evaporation and transpiration.

Finally, a mechanistic light-response (MLR) model driven by sun-induced chlorophyll fluorescence (SIF) was integrated into Daisy as an alternative to the standard Farquhar–von Caemmerer–Berry (FvCB) photosynthesis model. Since ecophysiological stress responses are embedded in the SIF signal, the MLR approach was expected to reduce parameter uncertainty and improve predictions. However, it did not outperform the FvCB model, which is likely due to the compounding uncertainties in SIF estimation and model assumptions. Both approaches underestimated photosynthesis during grain filling, pointing to a common structural weakness in representing non-foliar organ contributions.

Altogether, these three chapters constitute an integrated model assessment and development. It demonstrates both the potential and the current limitations of Daisy for simulating cropland flux dynamics under various conditions, while illustrating the mutual benefit of coupling process-based modelling tightly with targeted field observations.

Résumé

Les terres cultivées jouent un rôle central dans les cycles globaux du carbone, de l'azote et de l'eau, tout en figurant parmi les écosystèmes les plus vulnérables au changement climatique et aux phénomènes météorologiques extrêmes. Les modèles dits *process-based* sont un outil essentiel pour comprendre la dynamique des flux dans les cultures sous ces conditions, mais ils nécessitent une paramétrisation rigoureuse. Dans cette thèse, nous avons donc mis au point une méthode complète de modélisation (i.e., analyse de sensibilité, calibration et validation) et apporté des modifications au modèle sol-plante-atmosphère Daisy, pour son application aux cultures de blé d'hiver.

L'analyse de sensibilité globale portait sur l'évolution temporelle des échanges nets d'écosystème (NEE), de la chaleur latente (LE), de la chaleur sensible (H) et des flux de N_2O . Les sensibilités des paramètres ont montré des transitions marquées, associées aux stades phénologiques et aux conditions environnementales. Les paramètres photosynthétiques et stomatiques étaient prédominants pendant la croissance végétative, tandis que les paramètres hydrauliques du sol en profondeur étaient tout aussi influents lors des années humides, avec des conséquences sur toute la saison de croissance et soulignant la nécessité de mesures de terrain ciblées pour les sites mal drainés.

Daisy a ensuite été calibré par rapport à la matière sèche (DM), NEE et LE simultanément à l'aide d'un algorithme d'optimisation multi-objectif, puis validé. Cette analyse a révélé un compromis persistant entre DM et NEE, probablement dû à une sous-estimation de la respiration hétérotrophe, à des problèmes de paramétrisation dans le partitionnement du carbone ou à des biais systématiques dans les mesures par eddy covariance. Un problème d'équifinalité pour LE a également été identifié, pouvant résulter du découplage structurel entre évaporation du sol et transpiration.

Enfin, un modèle appelé MLR (*mechanistic light-response*) dépendant de la fluorescence émise par la chlorophylle (SIF) a été intégré à Daisy comme alternative au modèle de photosynthèse de Farquhar–von Caemmerer–Berry (FvCB). Vu que les réponses écophysiologicals au stress sont intégrées au signal SIF, l'approche MLR était censée réduire l'incertitude des paramètres et améliorer les prédictions. Ça n'a pourtant pas été le cas, probablement en raison des incertitudes liées à l'estimation de la SIF et aux hypothèses propres au modèle. Par ailleurs, les deux approches ont sous-estimé la photosynthèse pendant le stade reproductif, révélant un problème structurel commun dans la représentation des contributions des organes non foliaires.

Ensemble, ces trois chapitres constituent une évaluation intégrée et un développement du modèle. Ils démontrent à la fois le potentiel et les limites actuelles de Daisy pour la simulation de la dynamique des flux des terres cultivées, tout en illustrant l'intérêt mutuel d'un couplage étroit entre la modélisation *process-based* et des observations de terrain ciblées.

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Acronyms

Notation	Description
ABA	abscisic acid. 41
AOM	added organic matter. 37, 58
CBB	Calvin-Benson-Bassham. 27
DM	dry matter. 96, 98, 135
DS	development stage. 34, 59
EC	eddy covariance. 10, 116
EF	model efficiency. 106
ET	evapotranspiration. 117
FvCB	Farquhar, von Caemmerer and Berry. 130
GCM	general circulation models. 14
GHG	greenhouse gas. 3, 53
GPP	gross primary productivity. 12, 77, 130
GSA	global sensitivity analysis. 51–53
H	sensible heat flux. 10, 56
LAI	leaf area index. 42, 134
LE	latent heat flux. 10, 32, 56, 96, 98, 123, 131
LSA	local sensitivity analysis. 53
LSM	land surface models. 14
MLR	mechanistic light response. 20, 129, 131
MOO	multi-objective optimisation. 98
NBP	net biome productivity. 5
NEE	net ecosystem exchange. 12, 56, 96, 98, 131
NME	normalised mean error. 106
NPQ	non-photochemical quenching. 130
NSE	Nash-Sutcliffe efficiency. 54, 106
OM	organic matter. 58
PET	potential evapotranspiration. 35, 43, 116
PFT	plant functional type. 14
PLF	piecewise linear function. 76

Notation	Description
PQ	photochemical quenching. 130
REW	relative extractable water. 77, 159
RMSE	root mean square error. 54
rRMSE	relative root mean square error. 102
SA	sensitivity analysis. 53
SFM	spectral fitting method. 132
SIF	sun-induced chlorophyll fluorescence. 20, 77, 129, 131
SLA	specific leaf area. 57
SMB	soil microbial biomass. 37, 58
SMPSO	Speed-constrained Multi-objective Particle Swarm Optimisation. 98, 135
SOC	soil organic carbon. 10, 167
SOM	soil organic matter. 30, 37, 58
SSP	shared socio-economic pathways. 3
SVAT	soil-vegetation-atmosphere transfer. 14, 15, 34, 52, 54, 101
SWC	soil water content. 63
TPU	triose phosphate utilisation. 133, 143
VPD	vapour pressure deficit. 63, 97
WFPS	water-filled pore space. 7, 58
WSOrg	dry matter of storage organs. 61

1

Introduction

1. Global challenges

Agriculture is the major source of food and feed production and, to a lesser extent, fibre production. Our entire food systems heavily rely on arable lands, with 23.3% of food production, for example, consisting of cereals in 2023 (FAO, 2025a). As the main staple food worldwide, this represents more than 40% of our energy supply (FAO, 2025b). Cereals are even more essential for livestock and poultry feeding, constituting 66.9% of world feed production (FAO, 2025a). Nevertheless, food systems along with agriculture are at the heart of many global challenges. In 2024, it is estimated that 8.2% of the global population faced hunger (FAO et al., 2025). In the future, this percentage might even get worse due to the increase in food demand, predicted by the growing population, but also due to climate change (Becker and Fanzo, 2023). It is thus essential to better grasp all mechanisms and factors controlling cereal production in a changing world.

1.1. Climate change

Since the pre-industrial era (1750), the atmospheric concentration of carbon dioxide (CO_2) has increased from 278.3 to 415 ppm in 2021, corresponding to a gain of 49% (IPCC, 2023). Similarly, methane (CH_4) concentration increased by 160% and nitrous oxide (N_2O) concentration gained 24%. These three gases absorb and radiate heat into the atmosphere, causing radiative forcing and warming the Earth's surface. This phenomenon is commonly known as the greenhouse effect, hence these gases are referred to as greenhouse gas (GHG).

Global surface temperature has already increased by 1.15°C compared to 1850-1900 averages, with greater gains over land than over ocean (IPCC, 2023). Hot extremes, including heatwaves, have already strengthened in intensity, frequency and duration (Perkins-Kirkpatrick and Lewis, 2020; Yule et al., 2023), even faster than expected (Vautard et al., 2023). In their latest projections, the Sixth Coupled Model Intercomparison Project (CMIP6) predicts that temperature at the end of the century would be between 1.53 and 4.83°C higher than in 1850-1900 (Tebaldi et al., 2021). These predictions are based on five main shared socio-economic pathways (SSP) scenarios (Meinshausen et al., 2020). The lowest increase in temperature corresponds to SSP1-1.9, which is designed to limit warming to 1.5°C in accordance with the Paris Agreement. On the other hand, the highest increase refers to SSP5-8.5 which enacts an 8.5 W m^{-2} radiative forcing. If mitigation is not further implemented beyond what is currently in force, which is represented by SSP3-7.0, it is expected that temperature would increase by 2.30°C around 2050 and by 4.00°C at the end of the century (Tebaldi et al., 2021).

Additionally, the modification of Earth's energy budget is also expected to affect its hydrological cycle. As the atmosphere gets warmer, its moisture-holding capacity increases as well. This follows thermodynamic principles, and more precisely Clausius-Clapeyron equation, stating that saturated vapour pressure in the atmosphere rises by 7% per warming $^{\circ}\text{C}$ (IPCC, 2021). As a consequence, atmospheric vapour demand is enhanced and ultimately dries the land and vegetation, as observed since 1979 (Blunden and Arndt, 2019; Willett et al., 2014). This is compounded by the increase of vegetation transpiration in warmer atmosphere, as this process allows to cool vegetation surfaces. With more atmospheric water vapour, there is a higher potential for extreme precipitation and intense tropical storms (Trenberth, 2022). Moreover, as water is the major gaseous absorber in the atmosphere, it further strengthens the Earth's natural greenhouse effect. This acts as a positive feedback, amplifying the Earth's warming (IPCC, 2021). All these changes are often summarised as an *intensification* of the global water cycle.

As this is combined with potential changes in atmospheric circulation, projections of water cycle changes remain challenging. At a global scale, CMIP6 predicts a precipitation increase ranging from 2.02 to 7.30% for the end of the century compared to 1995-2014 (Tebaldi et al., 2021). The spatial and time distributions are however highly heterogeneous and subject to high uncertainty. For all scenarios, precipitation increases in wet areas but decreases in dry ones (Schurer et al., 2020; Deng et al., 2020). Depending on the region, it is then expected that drier days and intense precipitation events would be more frequent and intense, likely leading to more severe floodings and droughts (IPCC, 2021).

1.2. Cropping systems and GHGs

Due to these extreme events, agriculture is the most vulnerable sector to climate change. This is even more true for croplands, which are subject to frequent soil disturbances and consist mostly of annual crops that often have shallower root systems than perennials (grasslands and forests), making them less resilient to extreme events (Philipp et al., 2025; Basche and Edelson, 2017). This vulnerability is exacerbated by an expected increase in insect pests and diseases due to changes in temperature and weather patterns (Imtiaz et al., 2024). Nevertheless, cropping systems also contribute to climate change (Figure 1.1). Croplands absorb CO_2 through photosynthesis and release it during heterotrophic (microbial) and autotrophic (plant) respiration. These systems act as a nitrogen source, with an emission due to nitrification, denitrification and volatilisation of fertilisers greater than the atmospheric fixation. Finally, the CH_4 emission is due to production under anaerobic conditions, mainly observed in rice paddies (Serrano-Silva et al., 2014).

During 2007-2016, agriculture accounted for 40% of CH_4 and 79% of N_2O emissions from human activities (Jia et al., 2019). This is more balanced for CO_2 , as

agriculture encompasses both grasslands and croplands. While grasslands are usually reported as a carbon sink or neutral, croplands are mainly a source (Schulze et al., 2010; Prescher et al., 2010; Kutsch et al., 2010). The carbon budget of entire crop rotations, also called net biome productivity (NBP), depends on crop species, soil type and management practices (Yang et al., 2022). Some crop species generally act as a sink, such as winter wheat, spelt or winter barley, increasing soil carbon storage (Pique et al., 2020; Poyda et al., 2019). On the other hand, other crops like maize and soybean were reported as a net CO₂ source (Wang et al., 2015; Ranathunga et al., 2025).

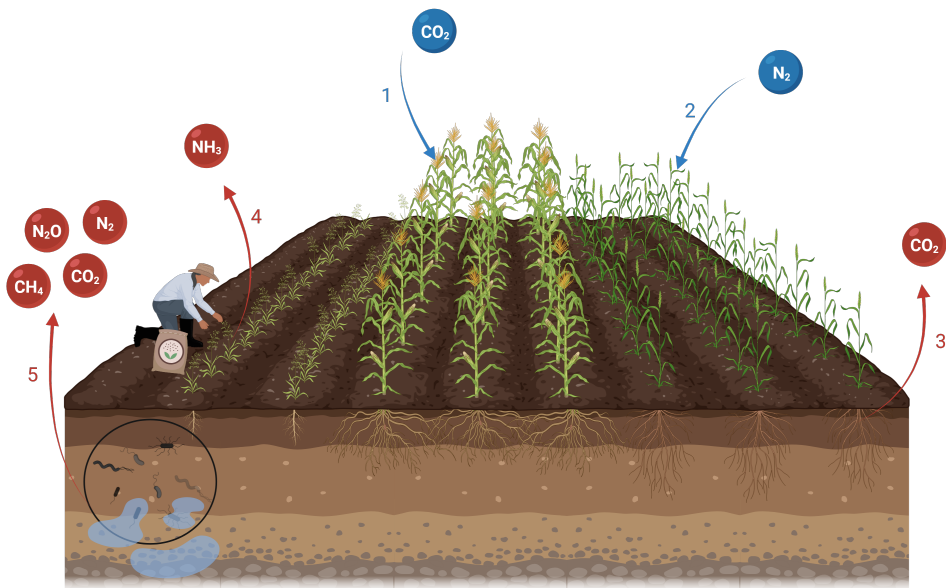


Figure 1.1: Greenhouse gases emitted and absorbed by croplands through (1) photosynthesis, (2) atmospheric fixation, (3) autotrophic (root and shoot) respiration, (4) volatilisation due to fertilisation, (5) heterotrophic respiration, loss during (de)nitrification and methanogenesis in anaerobic conditions.

As a consequence, even though agrosystems contribute to climate change, they also have a high potential for its mitigation. The most radical solution would be to convert croplands into grasslands or forests, resulting in better GHG budgets but further jeopardising food security (Miao et al., 2015; Wang et al., 2017). In a more reasonable way, several policy measures have been focused on agricultural soils in the past decades. In Europe, the “4 per 1000” initiative aims to increase carbon sequestration in soils (Soussana et al., 2019), the Farm to Fork strategy plans to reduce fertilisers application and nutrient losses (Montanarella and Panagos, 2021) and the recent – but

judged as lacking (Kotschik et al., 2024) – EU Soil Monitoring Law promotes the sustainable management of soils. In addition, the emerging EU Carbon Removals and Carbon Farming (CRCF) certification framework aims to create economic incentives for verified soil carbon sequestration (Hönle et al., 2026). These European orientations are increasingly relayed at the regional scale. Under the Common Agricultural Policy (CAP), agrienvironmental-climate measures (MAEC in French) reward farmers who have stored more carbon in their fields. They also reward practices with carbon sequestration co-benefits, such as sowing messicole plants around the cultivated parcels or even sowing strips of grasses and legumes to prevent soil erosion. In Wallonia, this is operated by Natagriwal, which advises and accompanies farmers in implementing such measures. The *Fédération Wallonne de l'Agriculture* (FWA) has engaged in similar efforts through its AgriClimate project (2025–2028), which conducts farm-level carbon audits and aims to help farmers valorise emission-reduction efforts. Besides these policy measures, researchers have been studying multiple solutions ranging from intermittent drainage for rice, reduced tillage and biochar application to changes in sowing dates, fertilisation timing and cultivars (Kabange et al., 2023; Malhi et al., 2021). For instance, the lack of synchronisation between crop nitrogen demand and supply is the main driver of N_2O emissions, with only 50% of applied nitrogen actually taken up by the vegetation (Jia et al., 2019).

2. Understanding crop flux dynamics

In order to accurately estimate the mitigation potential of croplands, it is essential to better understand these GHG and water fluxes as all of them contribute to climate change. More specifically, how the environmental conditions and extreme events can influence these flux dynamics. The various means to achieve this are described hereafter with some of their outcomes.

2.1. Experimental studies

Since long ago, researchers have designed experiments with controlled conditions. By enforcing future environmental conditions, such as elevated CO₂, higher air temperature or water-stressed conditions, they could observe and better understand the effects on crop dynamics. These experimental studies are thus essential for environmental science, but it is also worth noting that they often focus on specific conditions, as combining all of them is a tremendous task.

A widely known experimental study type is the Free-Air CO₂ Enrichment (FACE), where crops were cultivated under open-field conditions with elevated CO₂. They found that evapotranspiration decreased in these conditions, and yields increased or were unchanged depending on the water supply and the photosynthetic pathway (C3 or C4) of the crop (Kimball, 2016). This study portrays that changing a single environmental factor can affect the water use efficiency and, hence, the link between carbon and water cycles.

Under waterlogging conditions, net photosynthesis, transpiration and stomatal conductance were reported to decrease (Li et al., 2023; Kaur et al., 2020). These responses are mainly triggered by oxygen depletion in the rhizosphere, restricting root activity (growth and respiration) and causing an energy crisis. As a consequence, toxic metabolites accumulate which can result in cell death and plant senescence for prolonged waterlogging (Manghwar et al., 2024). Higher N₂O emissions were also observed under temporary waterlogging conditions, as well as lower soil respiration (Kemmann et al., 2023; Li et al., 2023). In parallel, Barrat et al. (2021) highlighted large but brief N₂O emissions, called hot moments, that were triggered by soil rewetting after edaphic drought. These moments depend on the water-filled pore space (WFPS) of the soil after rewetting, but also on the WFPS change between the dry and rewetted state. Barrat et al. (2021) suggested future studies to develop drought-impact curves, reflecting the relationship between N₂O emissions and drought duration or severity.

Leaf-scale (see Note 1 for more details) experimental studies also estimated the eco-physiological impacts of different environmental conditions on crops. Edaphic drought

was found to induce a decrease in leaf photosynthesis (-52.9%), transpiration (-51.8%) and stomatal conductance (-64.3%) of C3 crops, with a stronger decrease for higher drought intensity (Zhang et al., 2018; Yan et al., 2016). Maximum efficiency of photosystem II (referred to as $\Phi_{PSII,max}$ or F_v/F_m) decreased under moderate-to-severe droughts but not automatically under mild drought, even if it is associated with stomatal closure (Wang et al., 2016; Sommer et al., 2023; Pflüger et al., 2024). Heat was found to affect $\Phi_{PSII,max}$ even more (Pflüger et al., 2024), as it directly damages PSII structure by destabilising the oxygen-evolving complex and thylakoid membranes and indirectly inhibits PSII repairing (Allakhverdiev et al., 2008; Akter and Rafiqul Islam, 2017). Besides the damage to the photosynthetic apparatus, high temperature can also trigger a stomatal response. At high temperature, leaves open their stomata to enhance transpiration for cooling (Sato et al., 2024).

Under the combined effect of drought and heat, the impact of both stresses is increased (Zandalinas et al., 2018; Pflüger et al., 2024). Drought can be exacerbated by heat, which induces additional plant water consumption and soil evaporation. On the other hand, when stomata are closing under drought, it reduces transpiration and thus increases leaf surface temperature, worsening the heat stress (Sato et al., 2024). Under these combined conditions, plant responses can be challenging to predict. While heat and drought both negatively affect the photosynthesis, they have antagonistic effects on stomatal aperture (Zandalinas et al., 2016; Sato et al., 2024). Stomata tend to close under drought, to avoid water loss, whereas open stomata allow transpiration cooling. On another note, these antagonistic effects are also observed for soil respiration. Drought was reported to decrease both components of soil respiration, while heat was reported to increase heterotrophic respiration (Haghighi et al., 2021; Sun et al., 2019; Sippel et al., 2018).

Note 1: Overview of main leaf-level measurements

Gas exchange. Infrared gas analyser can be used to measure CO_2 and H_2O fluxes at the leaf level. To do so, leaves are enclosed in small chambers where specific light, humidity and CO_2 conditions are defined (Beauclaire, 2024). Once chamber conditions have reached equilibrium, leaf net CO_2 flux and transpiration can be measured, alongside leaf temperature and intercellular CO_2 concentration (Song and Zhu, 2024). The partitioning of the net CO_2 flux between photosynthesis and respiration components can be estimated later by darkening the leaf chamber (Beauclaire, 2024). Based on these measurements, it is also possible to determine the stomatal conductance and A/C_i curves.

Chlorophyll fluorescence. Energy absorbed by chlorophyll can either be used for photosynthesis, dissipated as heat or emitted as fluorescence. Thus, chlorophyll fluorescence (ChlF) can be defined as the light emitted by vegetation when electrons hopped from an excited to a non-excited state. Moreover, as the three processes (photosynthesis, heat dissipation and fluorescence emission) are complementary, ChlF has been widely used to probe photosynthesis (Kalaji et al., 2014). In experimental set-ups, ChlF emission can be induced with various techniques (pulse amplitude modulation, fast rise, fast repetition rate, etc.) and is commonly measured with fluorometers (Zavafer et al., 2020). These measurements allow to infer many physiological parameters such as the efficiency of photosystem II (PSII) or the fraction of open reaction centres (Beauclaire, 2024).

Leaf reflectance. Primarily used for phenotyping, spectroscopic techniques measured how leaves absorb and scatter light across wavelengths. Leaf traits (pigments, water and N content) and spectral indices such as the normalised difference vegetation index (NDVI) can thus be estimated. However, from the measurements of a spectroradiometer, photosynthetic variables can also be inferred using statistical models (Silva-Perez et al., 2018; Meacham-Hensold et al., 2019). These leaf variables include the maximum rate of carboxylation $V_{c,max}$ and the maximum electron transport rate J_{max} , which are both essential for photosynthesis.

All these leaf-level measurements can also be conducted at the ecosystem-level with different instrument setups. For instance, ChlF emission from the entire canopy can be estimated using a FloX tower. In this case, the measured emission would be directly induced by the sun instead of a predetermined light source, differentiating between passive and active techniques (Beauclaire, 2024). Hyper-spectral data can be collected at multiple scales, at the leaf-level or even using airborne or satellite (Grzybowski et al., 2021).

2.2. Monitoring croplands

While experimental studies provide essential insights on crop dynamics and responses under specific controlled conditions, these differ from real-life conditions. Indeed, many of these experiments focus on a few environmental factors and aim to reduce any other undesired factors, such as establishing optimal nutrient levels for studying the drought effect on crops. In an attempt to consider more factors simultaneously and get closer to reality, many ecotrons have been developed. These are controlled environment rooms where all weather and soil conditions can be recreated. However, in addition to considerable edge effects, real-life events such as storms, diseases or insect damage are hard to replicate. It is thus indispensable to monitor crops under real-life conditions as well.

Biomass measurements and phenological observations have been made for centuries to assess crop productivity and guide agricultural practices. Traditional methods for biomass evaluation are based on destructive measurements, making large-scale and long-term measurements time consuming. Easier but less accurate, non-destructive methods include allometric equations, remote sensing and proximal sensors (Wang et al., 2021). Similarly, soil organic carbon (SOC) and nitrogen content have been frequently measured since the 19th century to evaluate soil productivity (Ellert et al., 2007; Manlay et al., 2007). All these measurements provide static or periodic snapshots of crop and soil conditions, but limited information on fluxes. Even though repeated soil C inventories can quantify the C sink or source, eddy covariance (EC) is more complete and widely used for assessing ecosystem flux dynamics.

Originally developed in the 1950s to estimate evaporation from agricultural fields in Australia, EC has undergone significant advancements since the 1990s. These were facilitated by improvements in instrumentation, data storage and computing, and were encouraged by a growing interest in climate-related studies which require high-quality flux data (Hicks and Baldocchi, 2020). Nowadays, these systems provide direct and continuous measurements of fluxes, such as CO₂, sensible heat flux (H) and latent heat flux (LE) and, less frequently, CH₄ and N₂O (see Note 2 for more details). They are deployed globally across a wide range of ecosystems and are often part of FLUXNET or, in Europe, ICOS networks which make data standardised and freely accessible. Beyond the ecosystem level, these data can also be used with satellite remote sensing to produce global maps of carbon and water fluxes (Nelson et al., 2024; Baldocchi, 2020).

Note 2: Eddy covariance systems

Theoretical basis. Eddy covariance is based on the principle that vertical turbulent transport of a scalar quantity (e.g., CO_2 , H_2O , heat, momentum) can be determined as the covariance between its concentration and the vertical wind speed.

Instrumentation. For energy and gas transfer estimation, an EC system requires two core instruments mounted on a tower above the canopy: a three-dimensional sonic anemometer, which measures wind speed components and sonic temperature at high frequency (typically 10-20 Hz), and an infra-red gas analyser (IRGA) for the scalar of interest. Open-path analysers are placed directly in the air stream, while closed-path systems, as depicted in Figure 1.2, draw air through a heated tube to the analyser. Both types of analysers have their own advantages and drawbacks, please refer to Chapter 2 of Aubinet et al. (2012) for further details.



Figure 1.2: Eddy covariance system with a 3D sonic anemometer and a closed-path IRGA (BE-Lon).

Data processing and quality control. Raw high-frequency data require several corrections before fluxes can be computed. These include spike removal, coordinate rotation, spectral corrections and Webb-Pearman-Leuning (WPL) corrections (Aubinet et al., 2012; Burba, 2013). Periods of low turbulence, typically identified by the friction velocity (u_*) threshold, are excluded as they violate EC assumptions (i.e., fluxes are fully turbulent). The remaining gaps, which can represent a substantial fraction of the annual record, can be filled using standard approaches such as marginal distribution sampling (Pastorello et al., 2020).

Spatial representativeness. EC systems do not measure fluxes at a single point but integrate them over an upwind area called the flux footprint, whose size and shape depend on wind speed, wind direction, atmospheric stability and measurement height (Schmid, 2002). For cropland sites, this footprint typically spans 10^2 to 10^5 m^2 , meaning that the measured flux originates from potentially various surface conditions, depending on the level of heterogeneity within this area.

At the ecosystem level, carbon fluxes have specific terminology. The net CO₂ flux at the atmosphere-ecosystem interface is called the net ecosystem exchange (NEE). This is the sum of two opposite contributions: gross primary productivity (GPP) including photosynthesis and photorespiration, and ecosystem respiration (R_{eco}) which is equivalent to the dark respiration from all ecosystem components. Following the micrometeorological convention where downward fluxes are counted as negative and upward as positive, NEE is negative when more carbon is fixed than respired. As EC systems measure only the net CO₂ flux, multiple approaches exist to derive GPP and R_{eco} from NEE measurements. Daytime (Lasslop et al., 2010) and nighttime (Reichstein et al., 2005) partitioning are the most used approaches and are included in the ONEFlux pipeline (Pastorello et al., 2020) followed by FLUXNET and ICOS networks. More recently, several studies have developed partitioning approaches based on neural networks (Chen et al., 2024a; Tramontana et al., 2020).

When extreme events coincidentally occur at EC sites, it is thus possible to further analyse their impacts on measured and derived fluxes. Short-term heat extremes were found to increase R_{eco} and decrease GPP, reducing the sink potential of the ecosystem (Von Buttlar et al., 2018). In their review, they also reported that GPP and R_{eco} were slightly reduced under edaphic drought without heat stress. However, under the compound drought and heat events, GPP was strongly decreased while heat and drought impacts on R_{eco} partially offset each other (Von Buttlar et al., 2018; Schwalm et al., 2010). During such events, the decrease in GPP is sometimes accompanied by a decrease in water-use efficiency (WUE), defined as GPP/LE (Reichstein et al., 2007) or as yield/LE (Yan et al., 2025). It should be noted that these observations are focused on Europe, but plants can give contrasting responses depending on their photosynthetic pathway and the hydro-climatic conditions (Flach et al., 2018; Yang et al., 2016b).

Under normal conditions, N₂O emissions were found to be driven mainly by fertilisation, soil moisture, soil C content and temperature (Turco et al., 2026; Cowan et al., 2025; Lognoul et al., 2019; Gelfand et al., 2015; Huang et al., 2014). Under drought, N₂O emissions were reported to be reduced, as water was limiting, and unaffected by fertilisation (Gelfand et al., 2015). Conversely, they measured high emissions after intense rewetting events. Using automated chambers, increased N₂O fluxes were reported at the beginning of waterlogging before declining along with soil NO₃⁻ concentration (Anthony and Silver, 2021). As nitrification is limited under waterlogged conditions, it can also impact denitrification through NO₃⁻ availability if these conditions are prolonged.

2.3. *Process-based modelling*

Despite the wealth of knowledge provided by experimental studies and monitoring networks, both approaches have inherent limitations. As previously stated, the former are often constrained to specific conditions (growth stages, nutrient availability, spatial scales, etc.), while the latter are restricted to conditions currently observed. Moreover, EC systems cannot disentangle individual processes (e.g., GPP and R_{eco} within NEE). Models can address these limitations and offer a complementary framework. Process-based models are valuable tools for understanding the processes of the complex interactions in cropping systems (Rötter et al., 2018). By formalising our mechanistic understanding into mathematical equations, models allow processes to be isolated, scaled, extrapolated and tested under various conditions, even those that are difficult or impossible to observe directly.

Nevertheless, models are simplifications of reality, relying on many assumptions, thus disagreements between model outputs and observations are to be expected. Such disagreements are not necessarily failures but rather the starting point of model improvement (Silva and Giller, 2020). They help identify which processes are inadequately represented and need to be modified. Model improvement can be seen as a continuous cycle of simulations and experimentations, where simulations generate new hypotheses that guide targeted experiments and experimental results in turn refine model structure and parameterisation (Silva and Giller, 2020; Rötter et al., 2018).

2.3.1. **Brief history of model development**

The history of crop modelling dates back to the late 1960s, when pioneering work by de Wit (1965), Duncan et al. (1967) and Monteith (1965) laid the foundations for process-based descriptions of photosynthesis and dry matter accumulation (Jones et al., 2017; Boote et al., 2013). Early models such as SUCROS (van Keulen et al., 1982) and CERES (Ritchie, 1985; Jones et al., 1986) formalised the relationship between radiation interception, biomass production and phenological development. These were progressively enriched with soil water and nitrogen modules, making crop models more comprehensive but also more complex. In the 1990s, frameworks like APSIM (McCown et al., 1996), Daisy (Abrahamsen and Hansen, 2000) and DSSAT (Jones et al., 2003) emerged with a soil-centric cropping system perspective rather than crop-centric (Keating and Thorburn, 2018). With a focus on the soil, such frameworks can simulate complex systems, including intercrops, crop-livestock interactions and manure management. As justified by McCown et al. (1996): "*Crops come and go, each finding the soil in a particular state and leaving it in an altered state*". Since then, crop models (including cropping systems models) have been increasingly used across various fields of study (Keating and Thorburn, 2018). However, few significant improvements in process modelling were reported in the last 15-20 years, supposedly due to a lack of high quality field data (Keating and Thorburn, 2018; Rötter et al.,

2018).

In parallel, supported by climate modelling, the need to represent the land-atmosphere interface emerged in the 1960s. This interface is where mass, momentum and energy exchanges between the terrestrial biosphere and atmosphere take place. Implemented in general circulation models (GCM), early land surface models (LSM) were initially simple bucket models (Manabe, 1969) that were found to be inadequate (Verseghy, 2000). In the late 1980s, efforts were made by integrating multiple soil layers as well as an explicit vegetation layer in pioneering LSM (Pitman, 2003), namely SiB (Sellers et al., 1986) and BATS (Dickinson et al., 1986). Vegetation was categorised based on the concept of plant functional type (PFT), allowing to apply LSM at large spatial scales (Sato et al., 2015). Initially designed to capture the essential features of land-atmosphere interactions, LSM have progressively incorporated new (e.g., carbon cycling) and more realistic representations of the ecosystem. For instance, building on work by Farquhar et al. (1980), semi-mechanistic models of canopy photosynthesis-conductance were implemented in LSM (Sellers et al., 1996; Pitman, 2003). From then on, LSM were also called terrestrial biosphere models (TBM) in literature, emphasizing their biological and biogeochemical embedded processes. More recently, an increasing amount of additions have been made, including dynamic vegetation distributions, nitrogen and phosphorous cycling, fire and plant hydraulics (Fisher and Koven, 2020; Lawrence et al., 2019). Nowadays, landmark models such as CLM (Lawrence et al., 2019) and ORCHIDEE (Krinner et al., 2005) are routinely coupled to climate models and used to project future land-atmosphere feedbacks under different SSP scenarios (Boucher et al., 2020; Tebaldi et al., 2021).

Despite their parallel development, crop models and LSM have increasingly converged. Some crop models such as Daisy (Plauborg et al., 2010) and GECROS (Yin and Van Laar, 2005) have incorporated soil-vegetation-atmosphere transfer (SVAT) schemes (see Note 3 for further details) and biochemical photosynthesis modules (Farquhar et al., 1980), allowing them to simulate mass and energy exchanges in addition to agronomic outputs and management practices. Conversely, LSM have been coupled with dedicated crop models to better represent the specificities of managed ecosystems (e.g., harvest, intercrops, tillage and fertilisation) that standard PFT-based representations handle poorly. Notable examples are ORCHIDEE-STICS (De Noblet-Ducoudré et al., 2004), Agro-IBIS (Kucharik, 2003), T&C-CROP (Buckley Paules et al., 2025) and JULES-SUCROS (Van Den Hoof et al., 2011). These hybrid approaches reflect a broader recognition that neither crop models nor LSM alone are sufficient to capture the full complexity of crop dynamics.

Note 3: Soil-Vegetation-Atmosphere Transfer

Soil-Vegetation-Atmosphere Transfer (SVAT) schemes or models are tools for mathematical representation of the mass (i.e., water and CO₂) and energy transfer between the soil-vegetation continuum and the atmosphere (Oltchev et al., 1996). They essentially describe the physical and ecophysiological mechanisms of these exchanges.

What is the difference with LSM? The SVAT acronym has emerged from the hydrology and micrometeorology communities in the late 1980s to early 1990s (Shuttleworth, 2012). Originally intended to be one-dimensional at the field scale (Sellers et al., 1986), these models were also called land surface models by the climate modelling community when embedded in GCM (Pitman, 2003). These terms are now often used interchangeably (Shuttleworth, 2012), although strictly speaking LSM designates a model category, while SVAT can also refer to the mechanistic description of soil-vegetation-atmosphere exchanges independently of any specific model.

Theoretical basis of SVAT energy scheme. It adheres to the energy conservation of a system, which can be described as follows:

$$C_s \frac{\partial T}{\partial t} = R_n - H - \lambda E - G \quad (1.1)$$

where C_s is the heat capacity of the system, T the system temperature, R_n the absorbed net radiation, H the sensible heat flux (i.e., transfer of heat energy resulting in a temperature change with no phase change), λE the latent heat flux (i.e., transfer of heat energy due to a phase change, corresponding to evapotranspiration expressed as an energy flux via the latent heat of vaporization λ) and G the ground storage heat flux. This formulation is defined as *prognostic* because it explicitly models the thermal inertia of the system (leaf or soil surface layer) and the temperature is updated at each computing time step using differential equations (Sellers et al., 1986). In the *diagnostic* formulation, the system is assumed to be in thermodynamic equilibrium at any given instant, meaning that there is no thermal inertia nor storage during a time step. The budget can thus be solved iteratively and written as:

$$R_n - H - \lambda E - G = 0 \quad (1.2)$$

2.3.2. Gaps in simulating flux dynamics under extreme conditions

Although the historical trajectory outlined above shows that both crop models and LSM have grown increasingly comprehensive, their ability to reproduce crop responses under extreme or contrasting abiotic conditions remains less established than their ability to reproduce average or near-optimal conditions (Nóia Júnior et al., 2025; Heinicke et al., 2022). A growing body of model evaluation studies indicates that this is precisely where current models struggle most. Across an ensemble of 13 global gridded crop models, including ORCHIDEE-STICS and CLM-Crop, Heinicke et al. (2022) found that most models detected the occurrence of drought and heatwave events but underestimated their impacts on crop yield. The results were less positive when focusing on wheat under heat stress, where only six models detected the heatwave signal. This is supported by a global model intercomparison, including more than 30 wheat models such as Daisy, where simulated yields agreed reasonably well under moderate temperatures, but were less accurate as temperatures rose (Asseng et al., 2015a).

Kim et al. (2024) reached a comparable conclusion for excessive rainfall stress, showing that process-based crop models still fail to reproduce low yields under highly wet conditions. Focusing on waterlogging, a cross-model review examining 21 crop models identified persistent deficiencies in simulating capillary rise, crop resistance, crop recovery mechanisms and in the effects on soil nitrogen processes, phenology and yield components (Garcia-Vila et al., 2025).

These intercomparison studies therefore suggest that the main challenge is not simply to detect whether an abiotic stress occurs, but also to correctly represent the sequence of processes through which an extreme event propagates within the soil–plant–atmosphere continuum. Apart from the model fitting usually conducted with near-optimal instead of extreme conditions, another important difficulty arises from the fact that extreme conditions often affect several physiological and physical processes simultaneously. Drought, for instance, modifies soil water availability, plant water status, stomatal conductance, transpiration and photosynthesis, while heat stress simultaneously affects leaf temperature, vapour pressure deficit, photosynthetic capacity, respiration and transpiration (Yan et al., 2016; Sato et al., 2024; Pflüger et al., 2024). These processes are therefore strongly interconnected rather than acting independently. This is a reason why an accurate representation of the coupling between photosynthesis and transpiration is important when studying crop responses to abiotic conditions. Without such coupling, transpiration and photosynthesis are simulated through separate formulations, with no shared physiological drivers. A stress-induced change in stomatal aperture can then be reflected in the simulation of one flux without being consistently propagated to the other, so that the trade-off between carbon gain and water loss regulated by the plant is not captured. Simply implementing a coupling is, however, not sufficient for accurately simulating both fluxes. As mentioned before, LSM embedding such a coupling still failed to predict crop yield (Heinicke et al., 2022).

These results highlight that the fidelity of the coupling and the processes feeding it are also critical, not just its integration.

Another important modelling feature when simulating abiotic stress is the representation of soil water dynamics. Despite being central to drought and waterlogging responses, soil water movement is often described by simplified or empirical formulation in crop models, a limitation described by Jarvis et al. (2022) as "*the elephant in the room*" of crop modelling. Although these approaches can provide robust approximations for some applications, they do not explicitly represent soil water potential gradients and are therefore limited in their ability to reproduce upward water movement and capillary redistribution. Even Richards-based formulations, which provide a more physically consistent description of soil water flow, do not fully resolve the challenge of soil hydrology under extreme rainfall. Richards' equation primarily describes matrix flow, whereas structured agricultural soils can contain cracks, root channels and biopores through which water moves much more rapidly. This preferential flow can bypass a substantial fraction of the soil matrix and rapidly transport water and solutes to deeper layers (Beven and Germann, 2013; Jarvis, 2007).

It is within this respect that the Daisy soil-plant-atmosphere model, further described in Chapter 2, was selected for this thesis. As a hybrid framework combining a soil-centric crop model with an SVAT module, Daisy is comparatively well positioned to address the two challenges identified above. Its representation of soil water movement, including matrix and preferential flow, directly targets the soil hydrology weakness highlighted by Jarvis et al. (2022), while its SVAT-photosynthesis configuration (Plauborg et al., 2010) allows carbon and water fluxes to be simulated jointly and compared directly against eddy-covariance measurements. Daisy is not the only model with such characteristics, but additional reasons guided our choice. First, it can predict each component of carbon (GPP and R_{eco}) and energy (H and LE exchanged by the soil surface and vegetation) fluxes separately. Second, its hourly resolution is critical for capturing diurnal variability in fluxes and their responses to short-term environmental drivers. Third, it can simulate most of Belgian crop species as well as the agricultural practices commonly followed (ploughing, harrowing, etc.). Four, Daisy's open-source and modular character allows new process representations to be integrated and tested, which is not readily possible with several closed-source alternatives.

This choice is further supported by Daisy's extensive track record of applications. Initially published by Hansen et al. (1991) and substantially restructured over the following decades (Abrahamsen and Hansen, 2000; Hansen et al., 2012), Daisy has since been applied and documented in more than 120 peer-reviewed studies published between 2012 and 2025 alone (Holbak et al., 2026). This recent review confirms that Daisy reliably reproduces water balance, crop production, nitrogen cycling, carbon sequestration and the fate of agrochemicals across a wide range of climates, soils and management systems. Beyond single-model evaluations, Daisy has also been directly

benchmarked against other crop models in several European multi-model exercises. In a comparison of eight widely used crop models simulating winter wheat across 49 site-years in northwestern, central and southeastern Europe, Daisy achieved the best predictions of crop yield (Palosuo et al., 2011). In a similar comparison of nine crop models, on spring barley this time, Daisy was also among the models that performed best (Rötter et al., 2012). Most simulated crops are winter wheat, spring barley, potatoes and maize, but other minor crops have also been studied, such as sunflower, winter rye, common bean, white cabbage or oilseed radish.

Daisy has been widely applied in scenario analyses evaluating the effect of management and/or climate change on agricultural production and its environmental impact (Holbak et al., 2026). Such studies focus on crop production as well as water, nitrogen and carbon dynamics (Macholdt et al., 2020; Durand et al., 2018; Rasmussen et al., 2018; Zhou et al., 2018; Schwartzkopff et al., 2026; Pohanková et al., 2024). Besides scenario analyses, Daisy is still under active development, with recent implementation such as the diffusion-based root model that explicitly accounts for root mortality under waterlogged conditions or the mulch model that influences water and solute dynamics (Holbak et al., 2026; Vuaille et al., 2024).

The vast majority of these studies use the same version of Daisy. Closer to typical crop models, this version predicts photosynthesis with a simple light response curve and includes no SVAT module. Implemented in 2010, the Daisy-SVAT version that we selected has been significantly less evaluated. Seidel et al. (2016) compared these two versions in a field experiment conducted with common bean exposed to drought and heat stress. While both versions were equivalent under no stress conditions, they recommended to use the Daisy-SVAT version for drought and heat stress as it showed slightly better predictions under these conditions.

Daisy's soil, water and nitrogen modules, which are shared in both versions, are thoroughly validated. However, the SVAT module along its coupled carbon–water flux representation remains comparatively under-tested, particularly under contrasting or extreme abiotic conditions. This version was evaluated against measured soil water content, drainage flow, stomatal conductance and dry matter (Plauborg et al., 2010; Seidel et al., 2016; Motarjemi et al., 2021), but none of the reported applications benchmark Daisy-SVAT version against eddy-covariance measurements of NEE, H and LE. This leaves open how well the model captures the joint, sub-daily dynamics of these fluxes, and their potential decoupling, under various abiotic conditions.

With all this in mind, the overarching scientific problem addressed in this thesis can be formulated as follows: **How can a process-based soil-plant-atmosphere model be parameterised, evaluated and improved to reliably reproduce carbon, water and energy dynamics of winter wheat across contrasting abiotic conditions?** This problem is broken down into five research questions that we try to answer throughout this thesis:

1. Which processes and parameters actually control the simulated dynamics of cropland carbon, water and energy fluxes? (RQ1)
2. How does the relative influence of model parameters change under contrasting abiotic conditions and with crop development? (RQ2)
3. How can a process-based model be reliably parameterised using complementary observations of crop development and ecosystem fluxes? (RQ3)
4. To what extent can the simultaneous evaluation of biomass, carbon- and water-related fluxes reveal structural limitations that remain hidden when model outputs are considered separately? And, in connection with this question, under which conditions does Daisy fail to reproduce the joint behaviour of carbon and water exchanges? (RQ4)
5. Can an observation-driven alternative representation of photosynthesis improve the simulation of cropland flux dynamics? (RQ5)

3. Thesis objectives

The general objective of this thesis is to improve our understanding of the dynamics of carbon, water and energy fluxes in cropping systems, specifically in winter wheat which is the main staple food worldwide, under various abiotic conditions. This objective requires both a robust mechanistic modelling framework and high-quality field data to constrain it. Considering this, the thesis can be articulated around two main axes:

Axis 1: Development of a complete modelling workflow (i.e., sensitivity analysis - calibration - validation). Together, these three steps contribute to have fitted and robust results when applying Daisy on a study site. By revealing which processes or parameters are most sensitive and poorly constrained under normal and stressed conditions, it allows to assess if flux dynamics are accurately captured in these conditions and which part of the model can possibly be improved. Using advanced methods of sensitivity analysis and calibration, it can also give many insights on model structure, processes and parameters. Bearing this in mind, this axis specifically aims at conducting a global sensitivity analysis to identify the most influential parameters under various environmental conditions (Chapter 3), and at calibrating these parameters and validating Daisy against both flux and biomass measurements (Chapter 4).

Axis 2: Improvement of flux modelling. Instead of using common photosynthesis models, such as the empirical radiation use efficiency or the semi-mechanistic model based on Farquhar et al. (1980), a new approach was explored: the mechanistic light response (MLR) model (Chapter 5). Using sun-induced chlorophyll fluorescence (SIF) as a direct input to estimate GPP, a key advantage of this approach is that ecophysiological responses to environmental drivers are already embedded in the SIF signal itself, rather than being explicitly parameterised within the model. This reduces the uncertainty associated with the representation of stress responses in model structure and suggests a more direct and observation-driven link between measured canopy processes and simulated fluxes.

To enable a thorough modelling workflow (Axis 1), a comprehensive dataset is required, which should include high-quality flux data, biomass and soil measurements, phenology observations, meteorological monitoring and management information. Moreover, such dataset should cover multiple cropping seasons of winter wheat in order to have more robust results for the sensitivity analysis and calibration while keeping one season aside for validation. The ICOS station of Lonzée (BE-Lon) meets all these criteria and was chosen for this work. Monitored for more than 20 years, this site is a 4-year rotation cropland typical of central Belgium (Table 1.1) and provides

a long-term and comprehensive dataset of, notably, flux measurements acquired by an EC system. Furthermore, SIF measurements were conducted on this site in 2022, allowing to implement both above-mentioned axes on one single site, as depicted in Figure 1.3.

No process-based model simulating the above-mentioned fluxes with a sub-daily resolution has been routinely applied and calibrated for BE-Lon. To date, in previous modelling attempts, Hoyaux et al. (2008) and Beauclaire et al. (2023) focused on leaf gas exchanges, Buysse et al. (2017) on net carbon fluxes and Bachy et al. (2016), Bachy et al. (2018), and Bachy et al. (2020) on volatile organic compounds exchanges. Furthermore, Delandmeter et al. (2023) recently combined STICS outputs with carbon flux equations to simulate daily NEE and each of its components for a 16-year crop rotation. In a comprehensive way, Wu et al. (2016) applied ORCHIDEE-CROP for simulating GPP, NEE, LE and H fluxes, but for a single crop season (2006-2007) with no specific calibration.

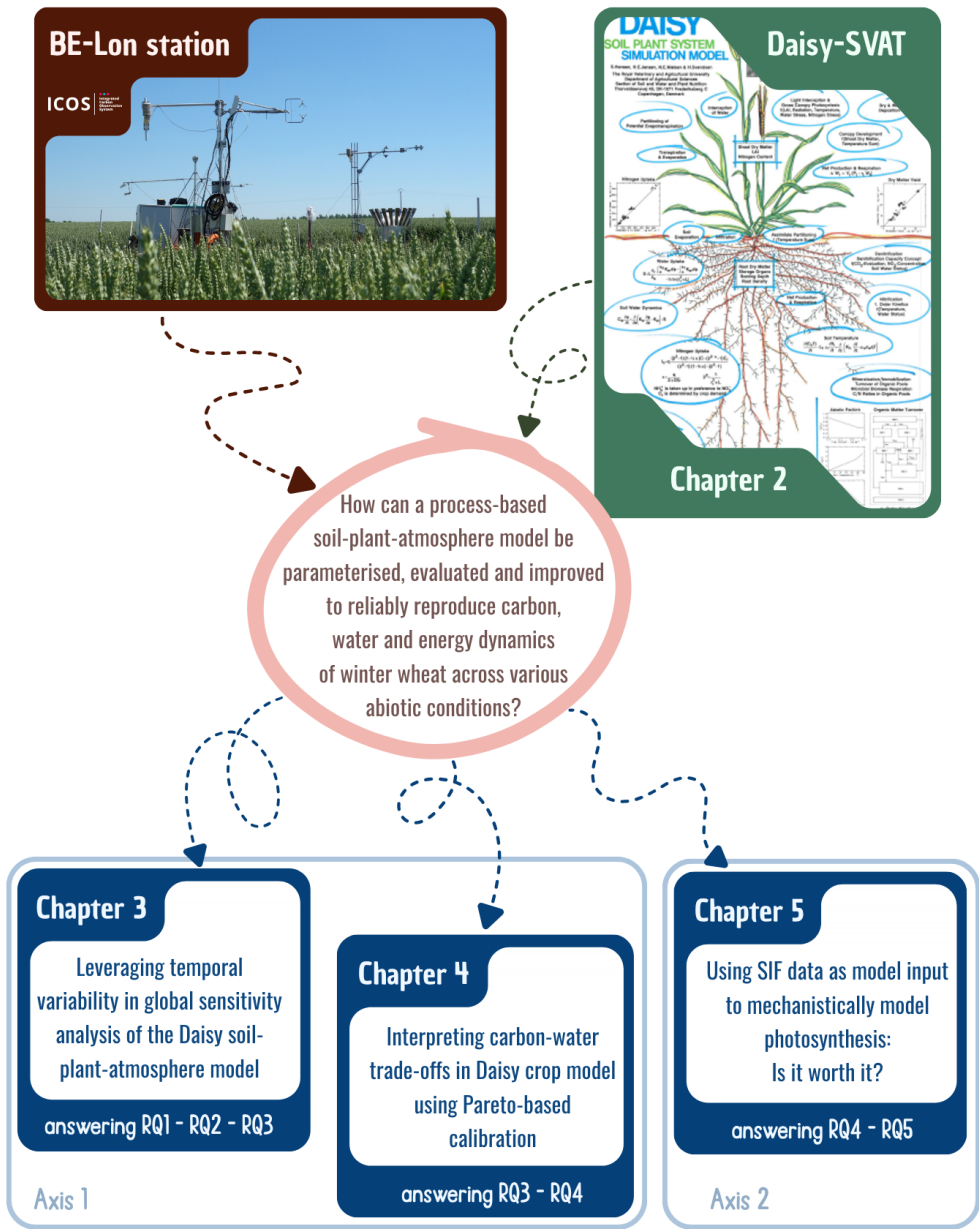


Figure 1.3: Thesis structure.

Table 1.1: Crop history in BE-Lon ICOS station. Crops in italics are cover crops. Yield ($\pm\sigma$) is expressed in tDM ha⁻¹ and represents tuber yield for sugar beet and potato, grain yield for winter wheat and ear yield for maize. Yield value indicated with * has not been directly measured.

Year	Crop	Sowing - Harvest	Yield
2004	Sugar beet	30 Mar - 29 Sep	18.96 $\pm$ 1.09
2004-2005	Winter wheat (cv. Dekan)	14 Oct - 03 Aug	8.95 $\pm$ 0.27
2006	Potato (cv. Spunta)	01 May - 15 Sep	7.49 $\pm$ 0.04
2006-2007	Winter wheat (cv. Rosario)	13 Oct - 05 Aug	7.5 $\pm$ 0.44
2008	Sugar beet	22 Apr - 04 Nov	24.46 $\pm$ 0.69
2008-2009	Winter wheat (cv. Ararat)	13 Nov - 07 Aug	9.16 $\pm$ 0.36
2009	<i>Mustard</i>	01 Sep - 01 Dec	-
2010	Potato (cv. Draga)	25 Apr - 05 Sep	7.92 $\pm$ 0.30
2010-2011	Winter wheat (cv. Sahara)	14 Oct - 16 Aug	9.16 $\pm$ 0.36
2012	Maize	14 May - 13 Oct	10.8 $\pm$ 0.70
2012-2013	Winter wheat (cv. Matrix)	25 Oct - 12 Aug	9.17 $\pm$ 0.14
2013	<i>Mustard</i>	05 Sep - 15 Nov	-
2014	Potato (cvs. Draga, Bianchidea, Kennebec)	07 Apr - 22 Aug	7.74 $\pm$ 1.34
2014-2015	Winter wheat (cv. Sahara)	14 Oct - 02 Aug	8.81 $\pm$ 0.19
2015	<i>Mustard</i>	21 Aug - 07 Dec	-
2016	Sugar beet	12 Apr - 27 Oct	23.64 $\pm$ 5.79
2016-2017	Winter wheat (cv. Tobak)	29 Oct - 30 Jul	8.63 $\pm$ 0.28
2017	<i>Mustard</i>	07 Sep - 07 Dec	-
2018	Potato (cvs. Draga, Unidea, Agria)	23 Apr - 11 Sep	10.31 $\pm$ 1.53
2018-2019	Winter wheat (cv. Smart)	10 Oct - 01 Aug	9.71 $\pm$ 1.27
2019	<i>Oat/Faba bean</i>	09 Aug - 03 Dec	-
2020	Sugar beet	01 Apr - 13 Nov	24.38*
2021	Spinach	01 Apr - 08 Jun	-
2021	Green dwarf bean	23 Jul - 24 Oct	-
2021-2022	Winter wheat (cv. Skyscraper)	28 Oct - 24 Jul	11.31 $\pm$ 0.45
2022	<i>Mustard</i>	13 Sep - 16 Nov	-
2023	Potato (cv. Cara)	03 May - 11 Sep	5.90 $\pm$ 1.35
2023-2024	Winter wheat (cv. Positiv)	16 Oct - 05 Aug	-
2024	<i>Phacelia/Clover</i>	31 Aug - 30 Nov	-

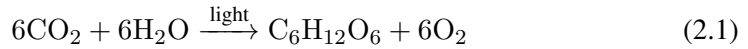
Cropland fluxes: Current knowledge and modelling tool

1. Key processes and drivers

Before introducing the modelling framework used in this thesis, we first review the main biophysical processes governing carbon, water and nitrogen cycles in cropping systems. These processes, together with their key environmental drivers, are considered successively at the leaf and soil level, with a focus on the exchanges with the atmosphere.

1.1. Leaf exchanges

Leaves are at the centre of two major gaseous fluxes: photosynthesis and transpiration. By absorbing CO₂ from the atmosphere, photosynthesis produces carbohydrates and dioxygen (O₂) according to this equation (Taiz et al., 2015):



This process includes light and carbon reactions, both intimately coupled. In C3 plants, light reactions produce NADPH and ATP that are used as chemical energy for the carbon reactions in the chloroplasts. These last reactions, improperly called dark reactions, consist of the reduction, carboxylation and regeneration occurring within the Calvin-Benson-Bassham (CBB) cycle (Sharkey, 2019; Taiz et al., 2015). Based on Equation (2.1), we know that photosynthesis depends on light absorbed by the leaves, on atmospheric CO₂ concentration and on available water. Furthermore, temperature affects all biochemical reactions of photosynthesis. As the temperature rises, there are two conflicting responses: an increase in the carboxylation rate and a decrease in the affinity of Rubisco with CO₂ (Taiz et al., 2015). Consequently, and also because the concentration ratio CO₂/O₂ decreases, photorespiration (i.e., oxygenation in the CBB cycle) is expected to increase as well (Ogren, 1984; Taiz et al., 2015).

For these photosynthetic processes to occur, CO₂ must diffuse from the canopy airspace into the chloroplasts. Using the resistance analogy from Ohm's law, the CO₂ flux is equivalent to the electric current. It is dependent on the CO₂ concentration gradient (i.e., voltage differential) and on the obstacles limiting the CO₂ diffusion (i.e., electric resistance). As depicted in Figure 2.1, the first illustrated obstacle is the leaf boundary layer resistance. It represents a thin layer of air surrounding each leaf, where fluid velocity decreases as a consequence of the friction with the surface and of fluid viscosity (Jones, 2014). A thick boundary layer can reduce the transfer of heat, mass (e.g., CO₂ and H₂O) and momentum between the canopy airspace and leaf surface. The leaf boundary layer resistance is mainly dependent on the wind speed and the leaf shape and size (Jones, 2014).

Secondly, CO_2 reaches the leaf intercellular airspaces by going through the stomata, which are microscopic pores in the leaf epidermis. Stomatal opening or closure is achieved by respectively increasing or decreasing the turgor in the guard cells compared to epidermal cells (Hikosaka et al., 2016). This process is driven by a lot of intricate environmental factors such as red and blue light intensity, soil water potential, air humidity, temperature, molecular signalling (like abscisic acid concentration) or atmospheric CO_2 (Jones, 2014; Buckley and Mott, 2013). As all these drivers can contribute concurrently, it is often difficult to predict the stomatal behaviour which can also differ between plant species (Merilo et al., 2014).

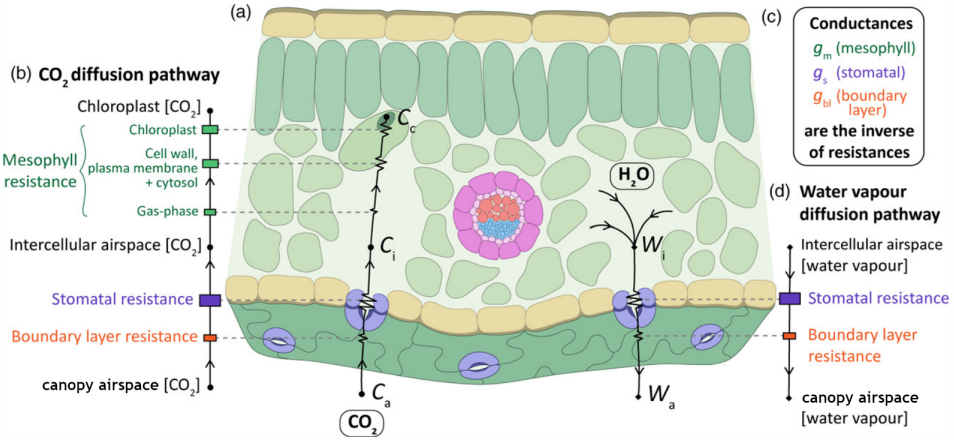


Figure 2.1: Pathway of diffusive resistances for CO_2 and water vapour in a C3 leaf from Harrison et al. (2020): Diagram (a) illustrating the route of gaseous exchange, and series of resistances along the (b) CO_2 and (d) water vapour diffusion pathway. C_a , C_i and C_c are respectively the CO_2 concentrations in the canopy and intercellular airspaces, and in the chloroplasts. Similarly, W_a and W_i are the water vapour pressures in the canopy and intercellular airspaces.

Before reaching the site of carboxylation in the chloroplasts, CO_2 has to go through a series of barriers that are encompassed and referred to as the mesophyll resistance r_m (Figure 2.1). It includes a gas phase component, several aqueous components and two lipid-protein components, making r_m a much more complex resistance than r_s (Gago et al., 2020). The mesophyll conductance¹ was reported to respond to CO_2 , light intensity, temperature, water availability and soil salinity, but the biochemical mechanisms driving these responses remain mostly elusive (Evans, 2021; Gago et al., 2020; Flexas et al., 2018).

Inside the leaf intercellular airspaces, water can be found in its liquid and gaseous forms. Liquid water comes all the way from the soil, moving through the roots and

¹As noted in Figure 2.1, the conductance of a component is the inverse of its resistance, these terms will both be used throughout this thesis.

xylem along a continuum of decreasing water potential (Bonan, 2019; Cochard, 2014). Once it reaches the leaf, airspaces become nearly saturated with water vapour which can ultimately be transpired (Cochard, 2014). By lowering the leaf water potential, transpiration can be seen as the force pulling water from the soil and driving plant hydraulics (Bonan, 2019; Jones, 2014).

From the intercellular airspaces to the canopy, the water vapour diffusion pathway is shared with CO_2 , making transpiration intrinsically linked to photosynthesis (Harrison et al., 2020). For instance, maximising the stomatal conductance g_s could increase the intercellular CO_2 concentration C_i and, hence, the chloroplast concentration C_c and photosynthesis would increase. However, it would also facilitate water vapour diffusion and induce an increase in transpiration, which illustrates the compromise between carbon supply and water loss in C3 plants. Conversely, C4 plants are less likely to experience this compromise due to their specific leaf anatomy and biochemical processes (Von Caemmerer and Furbank, 2016; Langdale, 2011). These plants have a high carboxylation efficiency and are less prone to CO_2 limitations, making them less dependent on carbon supply and better adapted to environments with high temperature and/or low atmospheric CO_2 (Kellogg, 2013).

Furthermore, CO_2 is also released by the leaves as a result of mitochondrial respiration. This respiration is also called dark respiration as it does not require light (Taiz et al., 2015), and autotrophic respiration when it is done by autotrophs such as plants. Along with CO_2 , this process produces adenosine triphosphate (ATP), which is the main source of energy for cells, and carbon skeletons that serve as building-block molecules for biosynthesis, nitrogen assimilation and maintenance (O’Leary and Plaxton, 2016; Atkin et al., 2010). Dark respiration rates vary greatly between species and depends on numerous environmental conditions such as temperature, water availability, atmospheric CO_2 and salinity (Aliyari Rad et al., 2022; O’Leary et al., 2019). Whereas some responses are more predictable, such as the temperature response, others require a better understanding of the underlying mechanisms (O’Leary et al., 2019).

1.2. Soil exchanges

1.2.1. Autotrophic carbon processes

Leaf respiration is not the only component of plant respiration. In the soil, living roots also release CO_2 as a by-product of high-energy molecules and/or carbon skeletons. Root respiration is controlled by soil temperature, water availability, salinity and partial pressure of CO_2 in the soil (Luo and Zhou, 2006). For instance, root respiration is restricted under waterlogged conditions (O_2 being limited), except for wetland plants that have evolved mechanisms of aeration (Manghwar et al., 2024; Luo and Zhou, 2006).

1.2.2. Heterotrophic carbon processes

Various substances are released in the zone surrounding these living roots, which is called the rhizosphere. It includes root exudates, sloughed-off cells, mucilage as well as dead root hairs, all being easily decomposable organic inputs (Cheng and Gershenson, 2007). Hence, the rhizosphere offers a highly favourable habitat for microorganisms (Luo and Zhou, 2006). The CO_2 produced by the activity of these microorganisms is known as the rhizomicrobial respiration. This is similar to the microbial respiration occurring outside of the rhizosphere during the decomposition of dead plant materials or other organic compounds. The only difference being that the organic matter is less labile compared to in the rhizosphere. Both of these components represent the heterotrophic respiration and are influenced by soil temperature, soil moisture, O_2 availability and the organic matter content and recalcitrance (Kuzyakov and Larionova, 2005).

1.2.3. Nitrogen processes

During the decomposition of soil organic matter (SOM), nitrogen can be mineralised. This mineralisation depends on several factors, notably the type of organic matter being decomposed, and can therefore be either positive or negative. The former means organic nitrogen is converted into ammonium (NH_4^+), which occurs when microorganisms have all the nitrogen they need. The reciprocal process is called immobilisation, when degraded SOM does not have enough N to meet microbial needs so microorganisms have to assimilate NH_4^+ from soil solution (Robertson and Groffman, 2024; Myrold and Bottomley, 2008). As depicted in Figure 2.2, ammonium is at the centre of numerous processes, being the interface between soil organic and other inorganic N forms, as well as between soil N and atmospheric ammonia (NH_3).

Ammonium can be converted into nitrites (NO_2^-) by ammonia-oxidising bacteria such as *Nitrosomonas*, and then into nitrates (NO_3^-) by *Nitrobacter* (Robertson and Groffman, 2024; Cameron et al., 2013). During these two reactions of nitrification, low amount of N_2O is generated as a by-product (Hofman and Van Cleemput, 2004). Furthermore, under anaerobic conditions, nitrates can be reduced into N_2O , nitric oxide (NO) and dinitrogen (N_2) during denitrification. Though less significant, this process can also take place in unsaturated soils and within soil aggregates, where oxygen diffusion is slow (Cameron et al., 2013). Both nitrification and denitrification are dependent on substrate supply, respectively NH_4^+ and NO_3^- , on soil moisture, microbial population and oxygen availability. When O_2 is limiting, nitrification would be restricted while denitrification would be enhanced (Robertson and Groffman, 2024). More specifically, in saturated soils, denitrification would occur until all nitrates are reduced, as production of NO_3^- is inhibited. On the other hand, in unsaturated soils, nitrification provides substrate for denitrification, which can be limited by O_2 or C availability. Soil carbon is also essential as it provides donor electrons to denitrifiers (Robertson and Groffman, 2024).

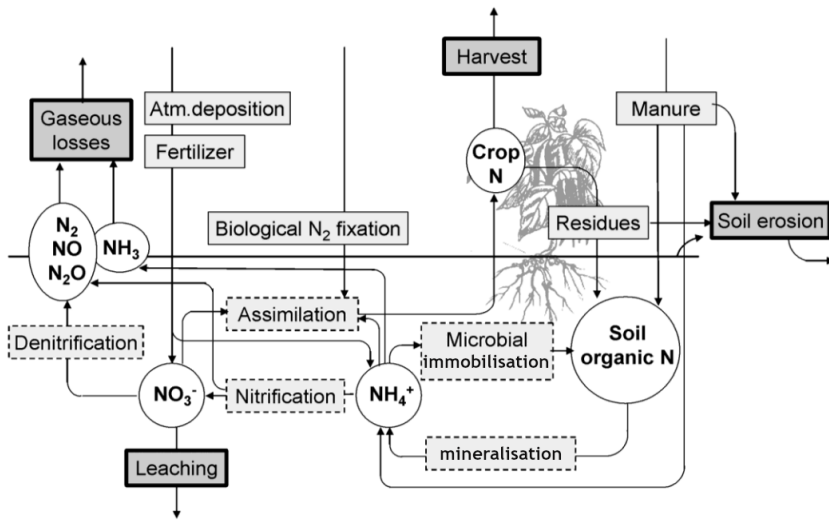


Figure 2.2: Nitrogen cycle in croplands adapted from Bouwman et al. (2009). Circles indicate pools, boxes with dashed lines are processes, light gray boxes with solid lines are inputs and dark gray boxes represent outputs.

Nitrates and ammonium are the two N forms easily assimilated by plants, although organic forms can also be accessed when mineral N supplies are limited (Schimel and Bennett, 2004). To improve nitrogen availability for plants, intensive agriculture heavily relies on organic and inorganic fertilisation. Inorganic fertilisers are mainly in the form of ammonium, ammonia, nitrates, urea, or a combination of these, while organic fertilisers encompass animal manure, sludge, plant-based fertilisers, etc (Hofman and Van Cleemput, 2004). Fertilisers use has numerous consequences on soil processes and exchanges. First of all, applied nitrogen can be lost into the atmosphere in the form of ammonia. This process, called volatilisation, can also be observed in unfertilised soil, as ammonium in the soil solution is in equilibrium with soil and atmospheric ammonia. However, much greater rates were observed following fertiliser application such as ammonium bicarbonate and urea (Cameron et al., 2013). Secondly, important NH_4^+ and NO_3^- concentrations can enhance nitrification and denitrification processes, increasing the emissions of N_2O . This is particularly the case when fertiliser amount does not meet the plant needs, being either excessive or poorly synchronised. Finally, depending on the soil drainage, nitrates can be leached from the rooting zone as they do not adsorb to negatively charged soil particles. They can ultimately reach groundwater, which is a serious threat to human health (Cameron et al., 2013; Hofman and Van Cleemput, 2004).

Besides fertilisers, nitrogen can be added into agrosystems through biological N fixation as well as wet and dry N deposition (Cameron et al., 2013; Reay et al., 2008).

Nitrogen fixation consists in the reduction of N_2 into ammonia NH_3 by diazotrophs (i.e., nitrogen-fixing microorganisms), which can be free-living or in a symbiotic association (De Bruijn and Hungria, 2022; Bottomley and Myrold, 2015). As it is an energy-expensive process, N_2 fixation mainly occurs in symbioses involving a photosynthetic host. A notorious example is the mutualistic relationship between rhizobia and legumes, noticeable by the root nodules. Rhizobia are supplied with carbon sources while making nitrogen assimilable for plants (Hofman and Van Cleemput, 2004).

1.2.4. Soil water processes

As described, all these processes are significantly impacted by soil water conditions and thus linked to the entire water cycle. The soil, being a porous material composed of solid particles, air, and water (Warrick, 2003), exhibits complex water movement depending on pore size, structure, and connectivity. Water is more or less likely to be infiltrated, percolated, absorbed by plants or evaporated based on these characteristics. When water from irrigation and rainfall reaches the canopy, it can either be intercepted by the leaves (and eventually evaporate) or reach the soil surface after dripping from leaves (throughfall) or flowing down the stem (stemflow) (Lin et al., 2020; Bellot et al., 1999). On the soil surface, water infiltration (i.e., downward entry of water into the soil) depends on soil characteristics and conditions. If the water supply exceeds the soil infiltration capacity, the remaining water ponds on the soil surface or runs off according to the local topography (Assouline, 2013).

In the soil, water movement occurs through two primary mechanisms: (i) matrix flow which is governed by gradients in soil water potential and dominates in smaller pores, and (ii) preferential flow where water moves rapidly through dynamic macropores (e.g., structural cracks, root channels, or other biopores), bypassing the soil matrix (Beven and Germann, 2013). High percolation rates can prevent waterlogging and anaerobic conditions, but can also leach more nutrients or pesticides into groundwater (Jarvis, 2007). Preferential flow accelerates this leaching and can create localised hotspots for microbial activities like denitrification (Jarvis, 2007; Bundt et al., 2001).

Evaporation from the soil surface constitutes a significant part of latent heat fluxes (LE), which is also composed of transpiration and evaporation from other surfaces. It is driven by the soil moisture availability as well as the atmospheric demand, which is the air vapour pressure deficit and depends on solar radiation, wind, air temperature and humidity. As for transpiration, the rate of soil evaporation depends on diffusion of water vapour through different airspaces and can be schematised with resistances along its diffusion pathway (Figure 2.3). Water vapour must diffuse across the water-air interface and through the dry airspaces before reaching the soil surface (Van De Griend and Owe, 1994). These soil resistances, often considered to be combined as one, are dependent on soil moisture and hydraulic properties (Bonan, 2019; Lehmann et al., 2018; Haghghi and Or, 2015).

As detailed previously (Section 1.1), the diffusion of water vapour through stomata lower the leaf water potential, propagating this gradient along the xylem and root segments. When the water potential is higher in the rhizosphere than in the roots, it induces an inflow of water from the rhizosphere (Lobet et al., 2014). This zone surrounding roots was reported to have different physical and chemical properties from the bulk soil, allowing to keep a high water content even during transpiration (Carminati et al., 2010). Furthermore, plants can adapt their root morphology and the quality and quantity of rhizodepositions to improve their water and nutrient uptake in dry conditions (Kost et al., 2026). At the root-soil interface, the rhizosphere is a critical zone under active research, impacting both soil processes and leaf-level transpiration (Cheraghi et al., 2023; Gregory et al., 2022; Carminati et al., 2010). It serves as a reminder that all these processes are tightly connected, even if these were separated into leaf and soil exchanges for the sake of clarity.

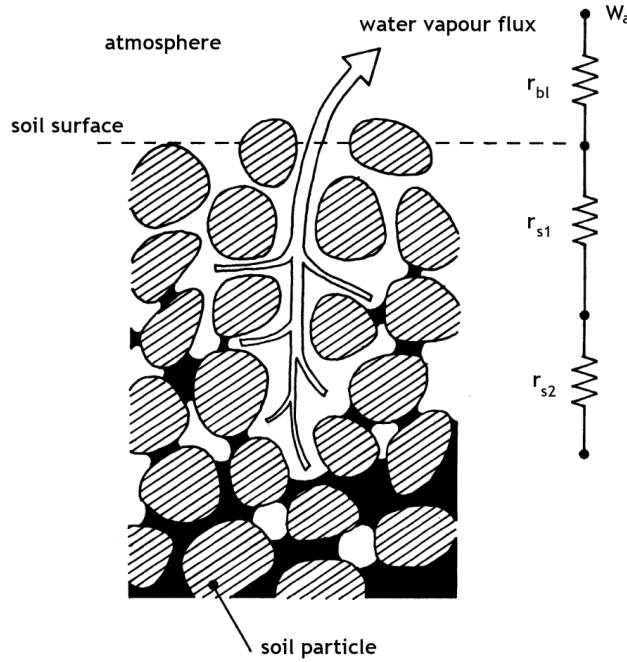


Figure 2.3: Pathway of diffusive resistances for water vapour in bare soil adapted from Kondo and Saigusa (1994). W_a is the water vapour pressure in the canopy airspace, r_{bl} the soil surface boundary layer resistance, and r_{s1} and r_{s2} the soil resistances in dry pores and across the water-air interface.

2. Daisy soil-plant-atmosphere model

This section introduces the Daisy soil-plant-atmosphere model, selected in this thesis to simulate cropland carbon, water, nitrogen and energy fluxes. We first present its general structure and the main modelling choices, before detailing how the atmosphere exchanges relevant to eddy-covariance measurements are represented.

2.1. Overview and key processes

Initially published by Hansen et al. (1991), Daisy² is a crop process-based model simulating carbon, nitrogen and water cycles of the soil-vegetation-atmosphere continuum (Figure 2.4). It operates at the field scale and integrates the physical, chemical and biological processes occurring in agricultural systems, all driven by meteorological conditions and management operations.

Daisy can be regarded as a modelling framework in which modellers have choices to make between different modelling options and process representations. For instance, the photosynthesis process can either be simulated with a simple light response curve (Hansen et al., 2012) or based on Farquhar et al. (1980) work. Similarly, the time resolution (hourly or daily) can be determined by the modeller depending on its objectives and data availability.

In this thesis, we used the 1D version of Daisy with an hourly time resolution. Furthermore, in order to enable comparison with EC measurements, we chose to include the soil-vegetation-atmosphere transfer (SVAT) module implemented by Plauborg et al. (2010). This module numerically solves the surface energy balance using a binary search algorithm, allowing the determination of leaf temperature as well as latent and sensible heat fluxes. To do so, the energy balance is coupled with the biochemical photosynthesis model, called FvCB after the authors' name of Farquhar et al. (1980), and with a stomatal conductance empirical model. In this configuration, minimal required inputs are hourly air temperature, air vapour partial pressure, global radiation, precipitation and wind speed.

The crop component, depicted at the interface between the soil and the atmosphere (Figure 2.4), is essentially composed of leaves, stems, roots and storage organs. Its development is characterised by a dimensionless scalar (called development stage (DS)) which progresses from 0 at emergence to 1 at flowering and reaches 2 at crop maturity. The progression rate of DS is governed by temperature sums and, depending on the crop, photoperiod. Throughout this development, the crop draws water and mineral

²Code documentation, model download and related publications are all accessible on this [website](#).

nitrogen from the soil via root uptake and accumulates biomass through photosynthesis. At the same time, CO_2 is released in the atmosphere as a result of autotrophic respiration, along with sensible heat due to air convection and latent heat (i.e., water vapour) through transpiration. It is assumed that transpiration is equivalent to the extraction of soil water by roots, meaning that no plant hydraulics is considered in Daisy. At harvest, part of aboveground (and belowground in case of tuber crops) biomass is removed from the system, while residues are incorporated back into the soil organic matter pool via biological processes or farming practices.

The soil, represented by the brown rectangle in Figure 2.4, is a central component which includes four interacting state variables: soil organic matter, soil mineral nitrogen, soil water and soil temperature. Application of organic fertilisers and incorporation of crop residues feed the organic matter pool, which is slowly decomposed within the soil. During this decomposition, organic carbon is mineralised in the form of CO_2 , released in the atmosphere, and organic nitrogen is converted into ammonium. The latter is dissolved in the soil solution and can be assimilated by the crop, immobilised once again or converted into nitrates (subject to crop uptake as well). During nitrification and denitrification, N_2O can be released into the atmosphere. Water enters the soil through infiltration of non-intercepted water, flows within the soil matrix according to Richards' equation and leaves through uptake, evaporation or percolation. When percolating, water can carry dissolved mineral nitrogen out of the profile; a process called leaching. All these processes are dependent on soil temperature which is determined based on vertical heat conduction and convection.

Potential evapotranspiration (PET) is an auxiliary variable computed using FAO56 simplified Penman-Monteith equation (Allen et al., 2006) and meteorological data. It is then partitioned into surface evaporation (i.e., intercepted by the crop canopy, by the litter layer or ponding at the surface), soil evaporation and crop transpiration. For each of these processes, it acts as a reference which may not be exceeded. In other words, actual evapotranspiration cannot be greater than the potential evaporative demand.

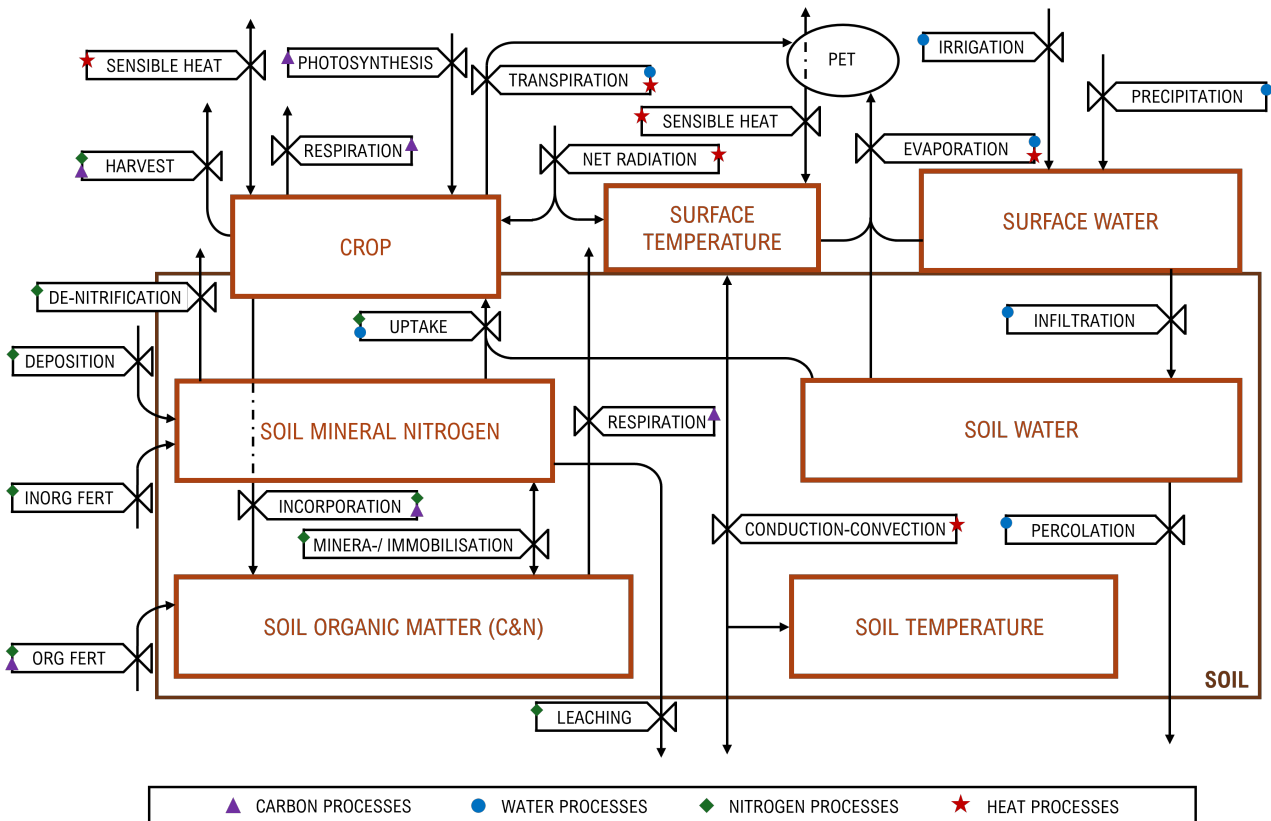


Figure 2.4: Daisy diagram - carbon, water, nitrogen and heat processes adapted from Hansen et al. (1991). Rectangles denote system main state variables, valve symbols indicate processes which are driving flows of matter (solid arrows) and ovals denote auxiliary variables.

2.2. Atmosphere exchanges

In this section, the atmosphere exchanges that are simulated by Daisy and measurable by EC systems are described in detail. These include the simulated processes of each flux components, such as photosynthesis, heterotrophic and autotrophic respiration for NEE, or surface evaporation and plant transpiration for LE.

2.2.1. Respiration

Microorganism respiration. Heterotrophic respiration arises from microorganism decomposition of organic matter in the soil. In Daisy, this organic matter is represented by a three-compartment model comprising the added organic matter (AOM) pools, which receive fresh crop residues and organic fertilisers, the soil microbial biomass (SMB) pools representing the living part of the soil (excluding roots) and the dead native SOM pools. Within each of these categories, organic matter is split into a slow-decomposing (denoted by 1) and fast-decomposing (denoted by 2) pools that have different turnover rates k . This is depicted in Figure 2.5 with indications of half-life in days or years, knowing that half-life is defined as $\frac{\ln 2}{k}$.

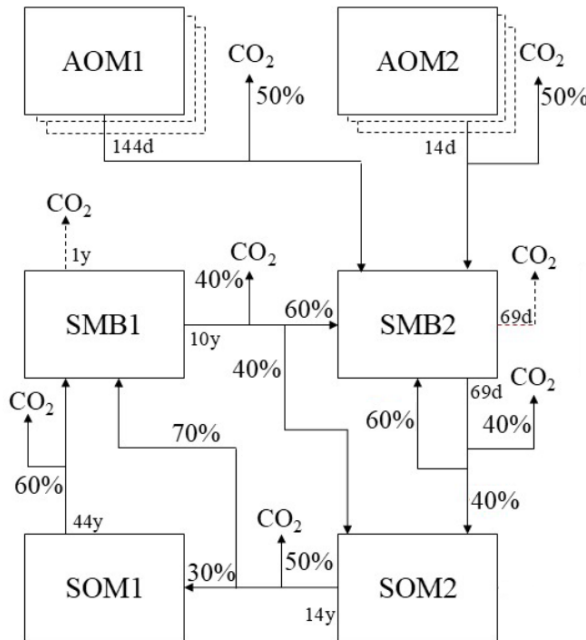


Figure 2.5: Organic matter module in Daisy adapted from their documentation.

CO₂ is released from both SMB pools due to their maintenance respiration, as shown by the dotted arrows, and during the breakdown of organic matter by these soil microorganisms, as depicted by the solid arrows. Carbon mineralisation rates are governed by first-order kinetics and turnover rates are affected by soil temperature, soil water content and, depending on the pool, clay content. CO₂ released by microorganism activity is directly emitted to the atmosphere and can be compared to carbon fluxes measured with EC systems when there is no vegetation in the footprint.

Plant respiration. In Daisy, autotrophic respiration is composed of maintenance respiration (R_m), growth respiration (R_g) and remobilisation respiration (R_r). Maintenance respiration R_m (gDM m⁻² d⁻¹) is the energy expenditure required to sustain existing biomass. Maintenance respiration is given priority over partitioning of new carbohydrates, so it is represented by a single arrow starting from the assimilate pool (Figure 2.6). It is, however, computed separately for each organ (leaves, stem, roots, storage organs):

$$R_m^{\text{org}} = r_m^{\text{org}} \cdot f(T) \cdot W^{\text{org}} \quad (2.2)$$

where r_m^{org} (d⁻¹) is the maintenance respiration coefficient of the organ, $f(T)$ is a temperature function and W^{org} is the organ dry weight (gDM m⁻²).

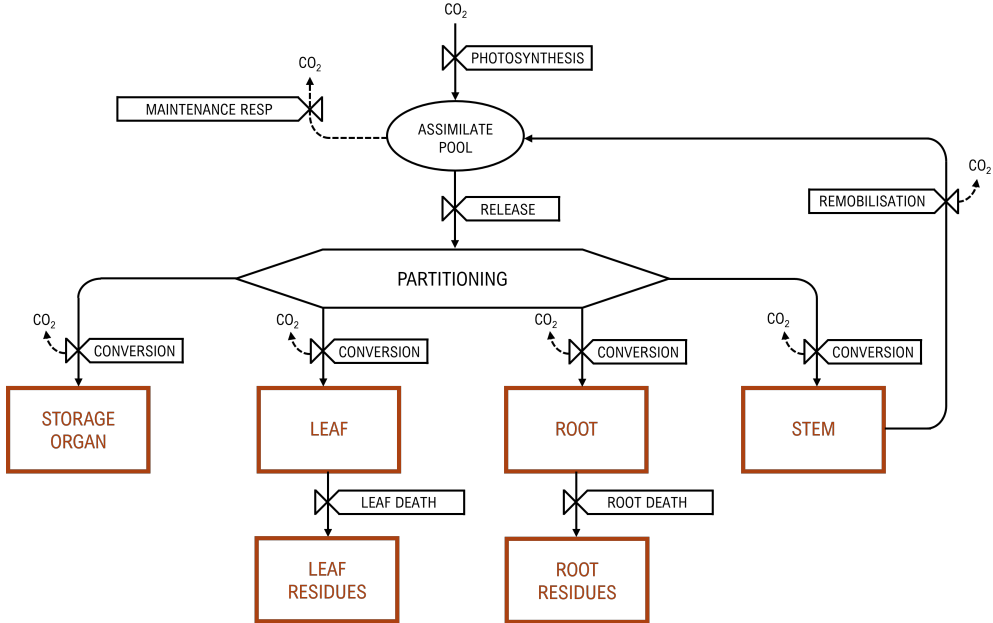


Figure 2.6: Crop carbon module in Daisy adapted from Hansen et al. (2012).

On the other hand, growth respiration represents the metabolic cost of converting assimilated carbon into new biomass. This respiration, along with production of new

biomass, only takes place if the available carbohydrates exceed the requirements for maintenance respiration. Growth respiration of an organ R_g^{org} (gDM m⁻² d⁻¹) can therefore be estimated as follows:

$$R_g^{\text{org}} = (1 - E^{\text{org}}) \cdot f^{\text{org}} \cdot F \quad (2.3)$$

where F (gDM m⁻² d⁻¹) is the total flux from the carbohydrates reserves, represented by the arrow pointing from the assimilate pool to the partitioning function (Figure 2.6), f^{org} is the fraction of assimilates allocated to the considered organ and E^{org} is the conversion efficiency.

Additionally, carbon reserves stored in the stem organ can be remobilised during the reproductive phase. Remobilisation is a first-order process which has a conversion cost of 15%, lost as CO₂ as depicted in Figure 2.6. This third respiration component R_r (gDM m⁻² d⁻¹) can be written as follows:

$$R_r = (1 - E_r) \cdot r_r \cdot f_r \cdot W^{\text{stem}} \quad (2.4)$$

where E_r is the conversion efficiency of remobilised reserves (0.85), r_r (d⁻¹) is the remobilisation rate, f_r is the fraction of stem that is considered as reserves and W^{stem} is the stem dry matter (gDM m⁻²).

In Figure 2.6, it is worth noting that the senescence of leaf and root organs does not release CO₂. Also described as a first-order process, the death rate of both organs is dependent on the crop development stage. Additionally, root death rate can be impacted by waterlogged conditions, but this parameter is not considered by default (nor in this thesis). Once dead, root carbon directly reaches the AOM pools (Figure 2.5) while leaf carbon either stay in the crop component, as dead material, or falls on the ground and will be gradually incorporated into AOM pools. Part of nitrogen contained in dead root and leaf is translocated to all organs upon death (respectively 10% and 90% by default).

The sum of these three autotrophic respiration components is subtracted from GPP to obtain net primary productivity (NPP). Total ecosystem respiration (R_{eco}) is then the sum of autotrophic and heterotrophic respiration, which, combined with GPP, yields the net ecosystem exchange ($\text{NEE} = R_{\text{eco}} - \text{GPP}$).

2.2.2. Gross primary productivity

Leaf photosynthesis. In the configuration used in this thesis, photosynthesis is simulated based on the biochemical FvCB model (Farquhar et al., 1980). It describes net leaf assimilation A_l as the minimum of two limiting rates; the Rubisco-limited rate (A_v) and the electron transport-limited rate (A_j):

$$A_l = \min \{A_v, A_j\} - R_l = A - R_l \quad (2.5)$$

where R_l is the leaf dark respiration rate ($\mu\text{mol m}^{-2} \text{s}^{-1}$). This equation assumes an abrupt transition between limitations (Figure 2.7). To address this issue, as more gradual transitions have been observed, Collatz et al. (1991) suggested to use a non-rectangular hyperbola:

$$\beta A^2 - (A_j + A_v) A + A_j A_v = 0 \quad (2.6)$$

where β is a curvature factor describing the transition between limitations, set by default to 0.95 in Daisy. When this factor tends to 1, A tends to $\min\{A_v, A_j\}$ as described in Equation (2.5).

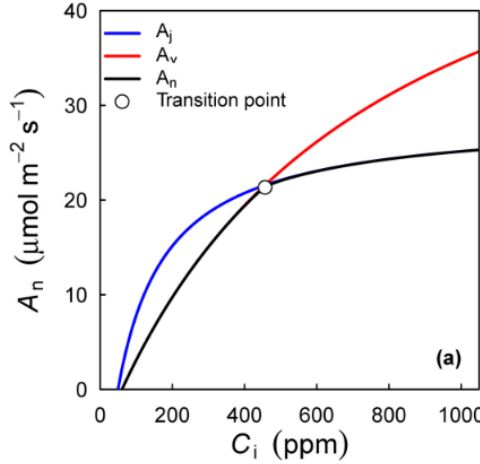


Figure 2.7: Limiting rates of assimilation in Daisy, taken from Duursma (2015), where A_n corresponds to A_l .

The first limiting rate A_v is proportional to the photosynthetic capacity of the RuBisCO enzyme V_1 and can be described as follows:

$$A_v = V_1 \frac{c_i - \Gamma_*}{c_i + K'} = V_1^{25} f(T) \frac{c_i - \Gamma_*}{c_i + K'} = \chi_n N_{\text{rub}} f(T) \frac{c_i - \Gamma_*}{c_i + K'} \quad (2.7)$$

where c_i is the intercellular CO_2 concentration, Γ_* is the CO_2 compensation point in the absence of mitochondrial respiration, K' is the effective Michaelis-Menten constant for the carboxylation, V_1^{25} is the photosynthetic RuBisCO capacity at 25°C , $f(T)$ is a temperature function from Bernacchi et al. (2001). As expanded in Equation (2.7), the photosynthetic capacity is expressed based on the leaf nitrogen content associated with photosynthesis N_{rub} and a model parameter χ_n representing the ratio between V_1^{25} and N_{rub} .

The second limiting rate A_j is also referred to as light-limited or RuBP regeneration-limited rate because it is dependent on the production of NADPH which can be related to PAR absorbed by the leaves (I_l):

$$A_j = J \frac{c_i - \Gamma_*}{4(c_i + 2\Gamma_*)} \quad (2.8)$$

$$\theta_1 J^2 - (\alpha I_1 + J_m) J + \alpha I_1 J_m = 0 \quad (2.9)$$

where J is the actual electron transport rate, θ_1 is a curvature factor, α is the fraction of absorbed PAR effectively reaching PSII and J_m is the potential electron transport rate, found to be proportional to V_1^{25} (de Pury and Farquhar, 1997). While the Equations (2.5), (2.7) and (2.8) are mechanistic, representing Rubisco kinetics in the CBB cycle and production of NADPH required for carbon fixation, the expression of J as a function of PAR is an empirical non-rectangular hyperbola (Von Caemmerer et al., 2025; De Pury, 1995). For this reason, FvCB is often qualified as semi-mechanistic.

On another note, it is worth mentioning that this leaf photosynthesis model considers the intercellular CO_2 concentration c_i instead of the concentration in the chloroplasts. It is assumed that the internal conductance to CO_2 diffusion from intercellular airspaces to the chloroplasts g_m is infinite. Leaf photosynthesis can thus be expressed as:

$$A_l = g_s(c_s - c_i) = (g_s + g_b)(c_a - c_i) \quad (2.10)$$

where g_s is the stomatal conductance, c_s is the CO_2 concentration at the leaf surface, g_b is the leaf boundary layer conductance and c_a is the CO_2 concentration in the canopy airspaces. The computation of the leaf boundary layer conductance for CO_2 is based on the conductance for heat (Section 2.2.4) and is fully described in the appendix C of Plauborg et al. (2010).

The stomatal conductance for CO_2 is simulated using Leuning formulation (Leuning, 1995) further adjusted for edaphic drought stress based on hydraulic signalling (Plauborg et al., 2010):

$$g_s = g_0 + \frac{g_1 \cdot e^{-\delta|\psi_c|}}{\left(1 + \frac{VPD}{D_0}\right) \cdot (c_s - \Gamma_*)} A_l \quad (2.11)$$

where Γ_* the CO_2 compensation point, VPD the vapour pressure deficit of the leaf surface, ψ_c the crown water potential (representing the plant water status and described by the related parameter δ) and g_0 , g_1 and D_0 are Leuning parameters. When δ is not null, stomatal conductance is reduced due to high crown water potential (in absolute terms). A second stomatal adjustment is implemented in Daisy, where g_s can also be reduced due to abscisic acid (ABA) concentration, and defined as chemical signalling. This second adjustment was not considered in this thesis as no ABA measurement was available.

Scaling up from leaves to canopy. Leaf-level gross assimilation must be integrated across the whole canopy to obtain a canopy-scale GPP that can be compared to EC-derived fluxes. In Daisy, this upscaling follows the layered two-leaf approach of de Pury and Farquhar (1997), which partitions the canopy both vertically (into layers of equal leaf area index (LAI) increment) and spectrally (into sunlit and shaded leaf fractions within each layer). To do so, a vertical profile for radiation, nitrogen and sunlit/shaded fraction needs to be estimated.

Radiation distribution. When going down into the canopy, all the solar radiation components are attenuated following Beer–Lambert’s law, described by an exponential decay. Based on their definition, radiation absorbed by the canopy I_c can be generally expressed as:

$$I_c = \int_0^{L_c} I_1 dL = (1 - \rho)I_0(1 - e^{-kL_c}) \quad (2.12)$$

where I_1 is the radiation absorbed by a canopy layer L and is integrated over the entire leaf area index of the canopy L_c , ρ is the leaf reflection coefficient, I_0 is the incident radiation above the canopy and k is an extinction coefficient.

In practice, incoming global radiation is decomposed into its direct-beam, scattered-beam and diffuse components, each with its own extinction coefficient. Scattered-beam radiation arises from single scattering of direct photons by leaves. Sunlit leaves absorb all three components, while shaded leaves only intercept the diffuse and scattered fractions, making sunlit leaves on average considerably more strongly irradiated under clear-sky conditions. In Daisy, this radiation partitioning is applied both to the PAR fraction of global radiation, governing leaf photosynthesis, and to the NIR fraction, required for the surface energy budget.

Nitrogen profile. Leaf nitrogen content associated with Rubisco, N_{rub} , is not uniformly distributed across the canopy. Upper well-lit leaves invest more nitrogen in the photosynthetic apparatus than lower shaded leaves, following a pattern of acclimation to the light environment that tends to maximise canopy-level carbon gain. In Daisy, this vertical gradient is described by an exponential decline with cumulative leaf area index L governed by a nitrogen extinction coefficient k_n :

$$N_{\text{rub}}(L) = N_{\text{rub},0}e^{-k_n L} \quad (2.13)$$

where $N_{\text{rub},0}$ is the value at the top of the canopy. Because $V_1^{25} = \chi_n N_{\text{rub}}$ (Equation (2.7)), both Rubisco capacity and the potential electron transport rate J_m decline with depth.

Sunlit and shaded fractions. The fraction of sunlit LAI in a canopy layer L decreases exponentially with the direct-beam extinction coefficient k_b :

$$f_{\text{sun}}(L) = \exp(-k_b L) \quad (2.14)$$

The complementary fraction $1 - f_{\text{sun}}$ represents the shaded leaves. Leaf photosynthesis (Equation (2.5)) is then evaluated separately for sunlit and shaded leaves in each canopy layer, using their respective absorbed PAR and the nitrogen content in that layer. Canopy GPP is finally obtained by summing leaf assimilation over all layers and both leaf fractions.

Numerical resolution. Because A_1 , c_i , c_s and g_s are mutually dependent, the equations cannot be solved analytically. Instead, an iterative solving method is used at each time step. Following Plauborg et al. (2010), the solution is structured around three nested iteration loops, each handling a different level of coupling.

The innermost loop resolves the coupling between c_i and A_1 within the photosynthesis component, keeping g_s and all other conditions constant. A_1 is expressed as a function of c_i through the FvCB model (Equations (2.6) to (2.9)) and c_i is in turn expressed as a function of A_1 through the diffusion equation (Equation (2.10)). By substitution, it is possible to get a single equation depending on c_i . As both functions constituting this equation are simple enough to derive, this loop can be solved using Newton–Raphson iteration and converges when the change in c_i between successive iterates falls below a fixed threshold.

The middle loop resolves the coupling between A_1 and g_s . Since g_s depends on A_1 (Equation (2.11)) and A_1 depends on c_i which is itself a function of g_s , the system is solved by successive substitution: the conductance estimated at iteration k is used to compute a new A_1 , c_i and c_s , which then yield an updated g_s and relative humidity at leaf surface h_s at iteration $k + 1$. Convergence is reached when the changes in c_i , h_s and g_s all fall below a fixed threshold.

The outermost loop couples the photosynthesis–stomatal conductance system with the SVAT module, which determines sunlit and shaded leaf temperatures T_{sun} and T_{shd} , canopy air vapour pressure e_c and actual transpiration by solving the surface energy balance (Plauborg et al., 2010). Because leaf temperature affects the temperature-sensitive parameters of the FvCB model (i.e., Γ_* , J_m and V_1), GPP and stomatal conductance are both affected by leaf temperatures. The conductance also influences latent heat flux, which feeds back into leaf temperatures, proving the two modules (A_1 – g_s and SVAT) are interdependent. Adopting a diagnostic formulation, this outermost loop is resolved using a binary search algorithm, and convergence is achieved when the changes in variables all fall below a fixed threshold.

2.2.3. Evapotranspiration

Potential evapotranspiration. Potential evapotranspiration (PET) constitutes the upper limit for the combined evaporative demand of all the ecosystem components. It is proportional to the reference evapotranspiration ET_0 specific to grass surface:

$$PET = K \cdot ET_0 \quad (2.15)$$

The coefficient K is used to convert the grass reference evapotranspiration to crop application. This coefficient is the sum of bare soil coefficient K_e and crop coefficient K_c , weighted by the cover fraction of each of these components. In the configuration used in this thesis, hourly vapour pressure and wind speed are available, so Daisy selects the Penman-Monteith formulation (Allen et al., 1998) to compute ET_0 :

$$ET_0 = \frac{0.03525\Delta (R_n - G) + \gamma \frac{0.9}{T+273} u_2 (e_s - e_a)}{24 \left(\Delta + \gamma \left(1 + \frac{r_{\text{surf}}}{r_a} \right) \right)} \quad (2.16)$$

Net radiation R_n (W m^{-2}) is computed from global radiation, air temperature, cloudiness and surface albedo, u_2 (m s^{-1}) is the wind speed at 2m height and the ground heat flux G (W m^{-2}) is derived from the simulated soil temperature profile. Δ (Pa K^{-1}) is the slope of the saturation vapour pressure curve, γ (Pa K^{-1}) is the psychrometric constant and $e_s - e_a$ (Pa) is the saturation vapour pressure deficit. r_{surf} (s m^{-1}) is the surface resistance, taken as 50 when net radiation is greater than zero, 200 otherwise (Allen et al., 2006), and r_a is the aerodynamic resistance, taken as $\frac{208}{u_2}$ (Allen et al., 1998).

PET is allocated sequentially to each aboveground component, acting as the driving demand, with each component consuming part of the remaining PET before passing it to the component below (Figure 2.8).

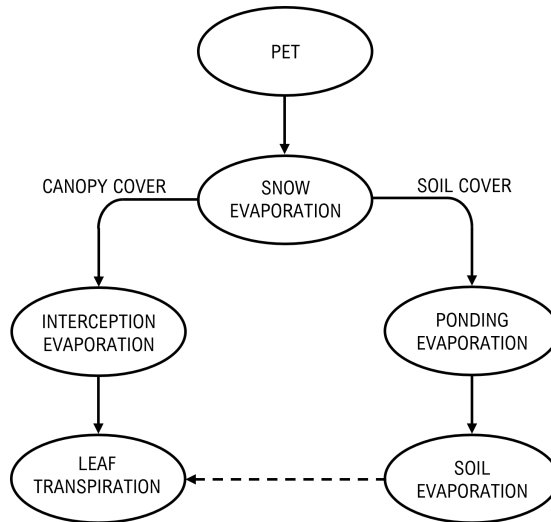


Figure 2.8: Distribution of potential evapotranspiration in Daisy.

Below PET, for each oval, the incoming arrow represents the potential evaporative demand allocated to this component. The outgoing arrow corresponds to the remaining potential demand which could not be met. When the soil evaporation cannot meet its

potential demand, 60% of the remaining PET is allocated to the crop transpiration, this energy transfer is depicted by the dotted arrow in Figure 2.8.

Evaporation. Precipitation intercepted by the canopy is stored up to a capacity proportional to LAI. Actual evaporation of this canopy interception is the minimum between the PET allocated to the canopy cover fraction and the available stored water. Any excess water beyond storage capacity reaches the soil as canopy drip-off (Figure 2.9).

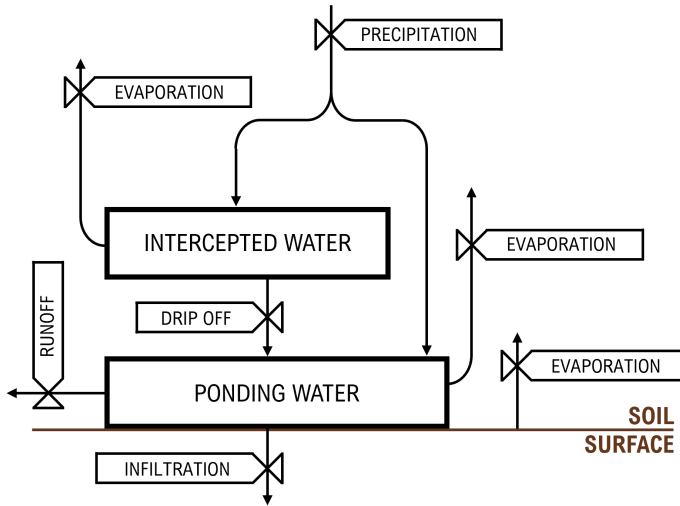


Figure 2.9: Overview of water surface processes in Daisy. This schematic view doesn't take snowpack, litter layer nor transpiration into account and irrigation is assumed to be included in precipitation.

Ponding occurs if water inputs exceed the surface potential evaporation and soil infiltration. In such case, the PET allocated to the soil cover is met if enough free water is available. Conversely, if the potential demand is still unmet, it is allocated to soil evaporation. Actual soil evaporation finally meets the remaining part of PET if it is not constrained by the rate at which soil water can be transported to the surface as computed by the soil water dynamics model.

Transpiration. Actual transpiration is determined in two steps. First, a soil-limited estimate is computed based on the ability of the root system to extract water from the rooting zone (Hansen and Abrahamsen, 2009) and is constrained by the potential transpiration. As depicted in Figure 2.8, potential transpiration is the sum of the PET not consumed by canopy interception evaporation and the transferred remaining PET from soil evaporation, redirected to the canopy. This soil-limited estimate serves as the initial guess for the SVAT iteration.

The SVAT module then refines this estimate through the outer iteration loop that couples actual transpiration with the photosynthesis and stomatal conductance computa-

tion described in Section 2.2.2. At each iteration, estimate of stomatal conductance g_s is given to the SVAT module, which resolves the surface energy balance for sunlit and shaded leaves and returns updated leaf temperatures, canopy air vapour pressure and a transpiration rate estimate. This transpiration rate is then used to update the crown water potential, which in turn updates g_s for the next iteration. Convergence is declared when the changes in T_{sun} , T_{shd} , e_c , boundary layer conductances and transpiration between successive iterations all fall below their respective fixed thresholds (by default 0.02 K, 1 Pa and 0.001 m s^{-1} 0.01 mm h^{-1}). The final actual transpiration is the minimum of the soil-limited and SVAT-limited estimates, ensuring that stomatal regulation can only reduce transpiration relative to what the soil can supply, not increase it.

2.2.4. Sensible heat

Sensible heat flux H (W m^{-2}) describes the transfer of heat between the ecosystem and the atmosphere by air convection. In the SVAT module, H emerges from the surface energy balance solved simultaneously for three sources: the soil surface, sunlit leaves and shaded leaves. For each source x , the sensible heat flux to the canopy air space is proportional to the temperature difference between that source and the canopy air (Plauborg et al., 2010):

$$H_{x \rightarrow c} = c_p \rho_a g_{x \rightarrow c}^H (T_x - T_c) \quad (2.17)$$

where c_p ($\text{J kg}^{-1} \text{ K}^{-1}$) is the specific heat of air, ρ_a (kg m^{-3}) is the air density, $g_{x \rightarrow c}^H$ (m s^{-1}) is the boundary layer conductance for heat of source x , and T_x and T_c are respectively the temperatures of source x and of the canopy air space. For sunlit and shaded leaves, $g_{x \rightarrow c}^H$ results from the combined effect of free convection, driven by the temperature difference between the leaf and the canopy air, and forced convection, driven by wind speed attenuated through the canopy. For the soil surface, a dedicated soil conductance accounts for wind speed conditions near the ground, which differ substantially from those at crop height (Plauborg et al., 2010). The total sensible heat flux to the atmosphere is then:

$$H_{\text{atm}} = c_p \rho_a g_a (T_c - T_a) \quad (2.18)$$

where g_a (m s^{-1}) is the aerodynamic conductance between the canopy air space and the reference height, and T_a is the air temperature at this height. g_a depends on vegetation height, LAI, wind speed and atmospheric stability through the Monin-Obukhov similarity theory (Plauborg et al., 2010).

Because T_{sun} , T_{shd} , T_c and T_{soil} appear simultaneously in the sensible heat, latent heat and radiation balance equations, these temperatures constitute the state variables of the SVAT system, along with the canopy air vapour pressure e_c . They are solved simultaneously at each time step from the five coupled energy balance equations of the soil, sunlit leaves, shaded leaves, total sensible heat and total latent heat (Plauborg

et al., 2010). This is what the outermost iteration loop described in Section 2.2.2 ultimately converges on: a physically consistent set of temperatures and vapour pressures that satisfies all five balance equations simultaneously given the stomatal conductances supplied by the photosynthesis model.

2.2.5. Nitrogen emissions

Nitrous oxide (N_2O) emissions in Daisy arise from nitrification and denitrification processes in the soil. Nitrification converts ammonium (NH_4^+) into nitrate (NO_3^-) and produces N_2O as a by-product at a fixed fraction (by default 2%) of the nitrification rate. This rate follows Michaelis-Menten kinetics with respect to total ammonium concentration:

$$\xi_n = V_n(T, h) \cdot \frac{N_{\text{am}}}{K_n + N_{\text{am}}} \quad (2.19)$$

where ξ_n ($\text{gN cm}^{-3} \text{ h}^{-1}$) is the nitrification rate, N_{am} (gN cm^{-3}) is the total ammonium concentration (sorbed and in solution), K_n is a half-saturation constant and $V_n(T, h)$ is the maximum nitrification rate modulated by temperature and soil water pressure potential.

On the other hand, denitrification is the biological reduction of nitrate to gaseous nitrogen species (N_2O and N_2). In Daisy, the potential denitrification rate is proportional to the CO_2 production rate estimated in the organic matter module, reflecting the dependence of denitrification on easily decomposable carbon as the electron donor (Lind, 1980):

$$\xi_d^* = f_d^T(T) \cdot \alpha_d^* \cdot \xi_{\text{CO}_2} \quad (2.20)$$

where ξ_d^* ($\text{gN cm}^{-3} \text{ h}^{-1}$) is the potential denitrification rate, ξ_{CO_2} ($\text{gCO}_2\text{-C cm}^{-3} \text{ h}^{-1}$) is the CO_2 production rate, α_d^* ($\text{gN gCO}_2\text{-C}^{-1}$) is a proportionality factor and f_d^T is a temperature function identical to that impacting $V_n(T, h)$ in Equation (2.19). The actual denitrification rate is the minimum between its potential rate and the rate limited by nitrate availability, which is assumed to be proportional to the nitrate concentration in the soil. Hence, the actual denitrification ξ_d can be expressed as:

$$\xi_d = \min \left(f_d^\theta(\theta) \cdot \xi_d^*; K_d \cdot N_{\text{NO}_3^- - \text{N}} \right) \quad (2.21)$$

where $f_d^\theta(\theta)$ is a soil water modifier function that acts as a proxy for anaerobic conditions, K_d (h^{-1}) is an empirical proportionality factor, reflecting the diffusion of nitrates to anaerobic sites, and $N_{\text{NO}_3^- - \text{N}}$ (gN cm^{-3}) is the nitrate concentration in soil. Although Daisy did not distinguish between N_2O and N_2 within denitrified nitrogen at the beginning of this thesis, a partitioning scheme has recently been implemented

based on Parton et al. (1996). This is a function of NO_3^- concentration, soil heterotrophic respiration and water-filled pore space, please refer to Daisy's technical documentation for further detail.

Leveraging temporal variability in global sensitivity analysis of the Daisy soil-plant-atmosphere model

Preamble. As a reminder, the general objective of this thesis is to understand carbon, nitrogen, water and energy fluxes of winter wheat crops through modelling using Daisy. Pursuing this objective requires that model behaviour be well comprehended before any attempt is made to tune it against observations. In this regard, the present chapter aims at assessing in a systematic and quantitative way which model parameters actually control model outputs and, more specifically, under which environmental conditions their influence varies. To do so, a global sensitivity analysis (GSA) was conducted on the Daisy configuration described in Chapter 2, targeting a combination of outputs for which observations are available at BE-Lon: crop yield, NEE, LE, H and N₂O emissions. This chapter also contributes to a broader methodological question in crop modelling: how should time-varying sensitivity be exploited to guide parameter estimation and reduce over-parameterisation? The findings reported here provided direct guidance on the choice of additional measurements, calibration targets as well as the parameter subspace later explored in Chapter 4.

For this third chapter, I developed the methodological framework for applying Morris and Sobol' methods on Daisy, performed the analysis of the GSA results and wrote the manuscript. Benjamin Dumont provided methodological advice and reviewed the manuscript. Bernard Longdoz supervised the research, contributed to the interpretation of the results and also reviewed the manuscript. It has been published as:

Delhez, L., Dumont, B., Longdoz, B.: Leveraging temporal variability in global sensitivity analysis of the Daisy soil-plant-atmosphere model, *Eur. J. Agron*, 165, 127533, <http://dx.doi.org/10.1016/j.eja.2025.127533>, 2025.

Abstract. Dynamic crop models, such as the Daisy soil-plant-atmosphere model, simulate many processes and encompass a large number of parameters. Global sensitivity analysis (GSA) aims to identify the most influential parameters and understand model structure and behaviour. However, little attention has been paid to the temporal dynamics of parameter sensitivity in crop models, even though it can provide greater insight into model structure. This study performs a comprehensive GSA on the Daisy model, including the soil-vegetation-atmosphere transfer (SVAT) module, focusing on crop yield as well as CO₂, N₂O and energy fluxes. The Sobol' method was applied to two types of outputs: (i) outputs aggregated into a scalar with an objective function (RMSE or cumulative) and (ii) vector outputs analysed at each time step. The main objectives of this paper were to compare the temporal and aggregated applications of GSA and to identify influential parameters of Daisy under different environmental conditions.

Both aggregated and temporal methods identified the same main parameters. Nevertheless, temporal analysis provided deeper insight into model behaviour and calibration guidelines, revealing dynamic changes in parameter sensitivity at weekly and hourly resolutions and identifying critical periods for calibration. Aggregated analysis was less time-consuming and focused on specific aspects due to the definition of the objective function. Finally, we discussed the risks and solutions for Daisy over-parameterisation as well as methods for parameter estimation based on information provided by the GSA.

1. Introduction

Over the past decades, crop models have been helpful tools to predict crop growth and yield while considering interactions with the environment (Asseng et al., 2014). They aim to improve scientific understanding and provide information for decision-making and policy support (Jones et al., 2017). Agricultural soils are significantly impacted by climate change and play a critical role in greenhouse gas (GHG) mitigation, so crop models have been developed to account for these dynamics. Many explicitly include the impacts of temperature, CO₂ concentration and rainfall variability on crop growth and yield (Asseng et al., 2015b). Furthermore, some crop models now incorporate more detailed process-based approaches, such as integrating energy balance or linking transpiration to carbon assimilation (Timlin et al., 2024). These enhancements provide a more accurate representation of soil-plant-atmosphere interactions and improve the prediction of GHG emissions.

As these crop models integrate more processes and require numerous parameters, sensitivity analysis (SA) is becoming a valuable first step in the modelling procedure, particularly for complex and over-parameterised models where many parameters can obscure critical inputs. Although this step is often overlooked, several authors have recently raised awareness about its importance (Saltelli et al., 2019; Seidel et al., 2018; Wallach et al., 2021). SA methods are now well established and provide useful insight into how a model responds to input factors and its underlying structure (Song et al., 2013; Massmann et al., 2014; Zhao et al., 2014; Razavi et al., 2021). Beyond model interpretation, SA is essential for prioritising key parameters for calibration, minimising uncertainty in model predictions, and guiding efforts toward refining influential parameters.

The main classification in SA techniques depends on how input factors vary in order to compute output variability. Local sensitivity analysis (LSA) explores the input space around a specific point by changing factors one at a time, whereas global sensitivity analysis (GSA) explores the entire input space with its interactions (Pianosi et al., 2016). Although LSA is easily interpreted and doesn't require a high computation cost (Song et al., 2015), it is unsuitable for nonlinear or non-monotonic models such as crop models (Saltelli et al., 2019). In contrast, GSA has received growing attention over the past 20 years, with derivative-based (Morris, 1991), variance-based (Saltelli et al., 2010) or density-based methods (Borgonovo, 2007; Pianosi and Wagener, 2018) being developed and improved. Comprehensive reviews on these methods can be found in Iooss and Lemaître (2015) and Pianosi et al. (2016). Derivative-based methods are referred to as qualitative and are often used as screening techniques before applying

computationally intensive methods to influential factors, such as variance-based methods (DeJonge et al., 2012; Sarrazin et al., 2016; Wang et al., 2018b; Stein et al., 2022).

Once a GSA technique is selected, the choice of output representation becomes crucial. Outputs for GSA are typically scalar functions, which are either a model prediction (e.g., crop yield at harvest) or an objective function assessing the model performance – such as the root mean square error (RMSE) or Nash-Sutcliffe efficiency (NSE) (Van Werkhoven et al., 2008; Shin et al., 2013; Wang and Solomatine, 2019). These objective functions aggregate temporal outputs into a scalar; a method hereafter referred to as aggregated GSA. However, the choice and definition of an objective function can significantly influence SA results, potentially covering interesting dynamic behaviour (Pianosi et al., 2016). This information loss, due to dimension reduction, is well documented (Wagener et al., 2003; Baddoo et al., 2020; Hodson et al., 2024) with some studies addressing it by using multiple objective functions (Van Werkhoven et al., 2008), applying different moving windows to temporal outputs (Medina and Muñoz, 2020) or using methods such as principal component analysis (Lamboni et al., 2009) or wavelet transforms (Bittner et al., 2021). Gupta and Razavi (2018) argue against the use of objective functions, suggesting that they focus on factor identifiability rather than true sensitivity analysis. They recommend computing sensitivity at each time step, resulting in a temporal GSA and limiting information loss.

Temporal GSA has been extensively applied in hydrology, where processes operate on multiple time scales (Massmann et al., 2014; Bittner et al., 2021), particularly in rainfall-runoff models (Cloke et al., 2008; Laloy and Bièlders, 2009; Kelleher et al., 2013; Pianosi and Wagener, 2016). Massmann et al. (2014) show that applying a temporal GSA several at time scales provides information on different processes. This technique is also relevant for agroecosystem models, as demonstrated by Song et al. (2013) with a forest model. Crop models that include more detailed processes can particularly benefit from temporal GSA. Whereas crop models initially simulate crop development on a daily time scale, integrating biochemical photosynthesis or energy fluxes leads to crop models having an hourly time step. As these processes act on different time scales, showing a high variability within a day and throughout the year, time-dependent parameter sensitivities can provide valuable insights into both diurnal and seasonal cycles. Such temporal insights are particularly useful for identifying critical periods when parameter uncertainties have the largest impact on outputs, helping modellers focus calibration efforts during these times.

In this paper, we applied both aggregated and temporal GSA techniques to a complex version of the crop model Daisy (Hansen et al., 2012), which includes a soil-vegetation-atmosphere transfer (SVAT) module (Plauborg et al., 2010). To our knowledge, no prior studies have directly compared these two GSA approaches within a crop model. This GSA was composed of a Morris screening method followed by a Sobol' variance-based method and was focused on crop yield as well as CO₂, N₂O

and energy fluxes, as the understanding of these flux dynamics is essential for climate mitigation. The main objectives of this paper were to compare the temporal and aggregated applications of GSA, illustrate how temporal GSA provides deeper insights into dynamic processes across different time scales, improve the understanding of Daisy model structure and behaviour, and identify influential parameters for more effective calibration.

2. Materials and methods

2.1. Case study

2.1.1. Site description

The study site, named BE-Lon, is a 12-ha cropland located in Lonzée, Belgium, that has been cultivated for more than 85 years. For at least two decades, a 4-year crop rotation typically found in the Hesbaye region has been adopted, i.e., winter wheat, seed potato, winter wheat, sugar beet. Farming practices are regarded as conventional with frequent 30-cm ploughing and the use of synthesised fertilisers and pesticides (managed according to integrated pest management principles). Manure from livestock is regularly applied to the plot. The climate is temperate maritime with an average annual temperature around 10°C and annual precipitation about 800 mm. Soil is identified as silt loam, which is well-suited to agriculture. It is composed of three main horizons: a ploughed surface horizon Ap, an intermediate horizon that can be classified as E (eluviated) or B (subsoil) across the plot, and a subsoil horizon with accumulated clays Bt.

Since 2017, this monitoring site has integrated the ICOS (Integrated Carbon Observation System) network as a Level 2 station. However, data have been recorded since 2004 as this station was previously a part of the CarboEurope project and already in the Fluxnet network. Additional information about the study site can be found in Buysse et al. (2017).

2.1.2. Measurements

As a Level 2 ICOS station, the site is equipped with an eddy covariance system continuously measuring CO₂, water vapour and sensible heat fluxes, referred to as net ecosystem exchange (NEE), latent heat flux (LE) and sensible heat flux (H). The sonic anemometer (Solent Research HS-50, Gill Instruments, Lymington, UK) is 2.4 metres above the ground and coupled with an infrared gas analyser (LI-7200, LI-COR, Lincoln, NE, US). The methodology described by Moureaux et al. (2006), Moureaux et al. (2008) and Aubinet et al. (2009) was applied to compute half-hourly flux data. Finally, data were postprocessed with the open-source code package ONEFlux to obtain derived-data products such as energy balance corrected fluxes (Pastorello et al., 2020). Aside from CO₂ and energy fluxes, two N₂O measurement campaigns were conducted on winter wheat crops. Data acquisition as well as flux computation and treatment are described in Lognoul et al. (2019).

Additionally, a micrometeorological station delivers data on a half-hourly basis. This

includes air temperature, relative humidity, different components of solar radiation and precipitation. These measurements are complemented by phenology observations along with vegetation and water table depth measurements. Throughout each growing season, biomass of leaves, stems and storage organs (referred to as WSOrg) is measured at least 7 times. Simultaneously, measurements of vegetation height and green area index are made, and phenology stages are estimated according to the BBCH scale. Finally, once per growing season, a measure of specific leaf area (SLA) is carried out around anthesis.

2.1.3. Crop management

Data were collected over four growing seasons of winter wheat (*Triticum aestivum* L.), which is the most cultivated cereal grain in Belgium. Management actions for each variety are summarised in Table 3.1. In Belgium, winter wheat is usually sown between mid-October and late November. Soil preparation was performed with a rotary harrow. Nitrogen fertilisation is commonly split into three applications to meet plant needs: the first application happens during the tillering stage in early spring, nitrogen is applied a second time near the beginning of stem elongation (BBCH 30) and a third time at flag leaf stage (BBCH 37-39) (Dumont et al., 2015a; Dumont et al., 2015b).

Table 3.1: Management activities of winter wheat crops in BE-Lon. Amount of nitrogen application is expressed in kgN ha⁻¹ and grain yield in tDM ha⁻¹.

Name	Variety	Date	Action	Amount
SAH	Sahara	14-10-2014	soil preparation + sowing	-
		14-03-2015	N application (liquid)	58.5
		15-04-2015	N application (liquid)	39
		11-05-2015	N application (liquid)	81
		02-08-2015	Harvest (grain yield)	8.81
TOB	Tobak	29-10-2016	ploughing + soil prep. + sowing	-
		16-03-2017	N application (liquid)	68.25
		12-04-2017	N application (liquid)	39
		12-05-2017	N application (liquid)	68.25
		30-07-2017	Harvest (grain yield)	8.63
SMA	KWS Smart	10-10-2018	soil preparation + sowing	-
		25-03-2019	N application (liquid)	58.5
		17-04-2019	N application (liquid)	39
		20-05-2019	N application (solid)	81
		01-08-2019	Harvest (grain yield)	9.71
SKY	LG Skyscraper	28-10-2021	ploughing + soil prep. + sowing	-
		24-03-2022	N application (liquid)	58.5
		14-04-2022	N application (liquid)	39
		17-05-2022	N application (solid)	54
		24-07-2022	Harvest (grain yield)	11.31

Although Table 3.1 shows similarities in management activities, four different wheat varieties were sown. In terms of precocity, the varieties TOB and SKY are identified as mid-late and are known to reach heading stage (BBCH 55) faster than the varieties SAH and SMA considered to be late cultivars. Regarding maturity (BBCH 89), TOB and SKY are characterised as mid-early while others are defined as late to very late (Meza et al., 2018; Meza et al., 2023).

2.2. Model description

Daisy is a crop model that has been fully described in the literature (Abrahamsen and Hansen, 2000; Hansen et al., 2012). This model simulates the carbon, water and nitrogen cycles of the soil-vegetation-atmosphere continuum, subsequently estimating the fluxes of CO_2 , H_2O and N_2O . In Daisy, this one-dimensional continuum is called the column component. Depending on data availability as well as the modeller's objectives, the processes involved in this component can be simulated with different levels of complexity and time resolution (hourly or daily). The adopted version and parameterisation of Daisy are briefly described hereafter.

2.2.1. Soil

Three types of organic matter (OM) are established in Daisy: plant residues or added organic matter (AOM), soil microbial biomass (SMB) and non-living soil organic matter (SOM). They either have a slow or fast mineralisation rate, resulting in six OM pools. Organic nitrogen is tightly linked to OM pools through their user-defined C/N ratio, and mineralisation or immobilisation of nitrogen takes place to maintain their ratio. In the soil solution, nitrification and denitrification processes depend on environmental conditions such as soil temperature and humidity. N_2O is lost as a constant fraction of NH_4^+ during nitrification. Nitrogen is also lost during denitrification, but Daisy doesn't distinguish between N_2O and N_2 . To address this, we estimated the ratio $\text{N}_2\text{O}/(\text{N}_2\text{O}+\text{N}_2)$ $f_{\text{N}_2\text{O}_{\text{denit}}}$ based on STICS (Brisson et al., 2009) formalism and depending on soil pH, water-filled pore space (WFPS) and NO_3 concentration (Léonard, 2016):

$$f_{\text{N}_2\text{O}_{\text{denit}}} = r_{\text{cor}} \cdot \left(1 - \frac{\text{WFPS} - l}{1 - l} \right) \cdot \frac{\text{NO}_3}{\text{NO}_3 + 1} \quad (3.1)$$

where r_{cor} is based on soil pH (equal to 0.66) and l is the threshold of WFPS above which denitrification starts to be active (set to 0.62). Although the effects of environmental factors on this ratio remain poorly understood (Zhang et al., 2023), this addition allows us to consider N_2O emitted from both processes and enables comparison with measurements.

Water movement in unsaturated soil is described by Richards' equation and, for each soil layer, retention and conductivity curves have been established with the Mualem-van Genuchten model (Mualem, 1976; van Genuchten, 1980). Drains, located at a

depth of 70 cm, are explicitly considered in the column component and water flow toward the drain is based on Hooghoudt theory (Mollerup et al., 2014). Moreover, an aquitard layer (i.e., water blocking layer) is situated below the soil profile.

2.2.2. Vegetation

Vegetation is schematised by four compartments: root, leaf, stem and storage organs, all of them containing a carbon content proportional to their dry matter content and a nitrogen content depending on their demand and availability of NO_3^- or NH_4^+ . In this version, photosynthesis is simulated by a biochemical model (de Pury and Farquhar, 1997) implemented by Plauborg et al. (2010), rather than by a light response curve also included in Daisy. This model (hereafter FvCB) determines photosynthesis of sunlit and shaded leaves based on the regeneration of RuBP and the availability of Rubisco. To estimate the intercellular CO_2 vapour pressure (required for FvCB), it is coupled with the stomatal conductance model proposed by Leuning (1995). Autotrophic respiration is due to maintenance of existing dry matter and conversion of new assimilates into dry matter. Partitioning of assimilated dry matter to the plant compartments is based on development stage (DS) but can be regulated by the shoot nitrogen status (Gyldengren et al., 2020). Development rate of the vegetative phase, from emergence (DS=0) to anthesis (DS=1), is based on a reference rate (DSRate1) which is influenced by temperature and photoperiod while only temperature affects the development of the reproductive phase (DSRate2), from anthesis to maturity (DS=2).

2.2.3. Energy balance

The SVAT module (Plauborg et al., 2010) estimates the surface energy balance to compute sensible heat, latent heat and radiative fluxes, as well as surface temperature. Incoming shortwave and longwave radiation are respectively given to Daisy as inputs and estimated based on the Brunt (1932) model. The diffuse fraction within global radiation as well as vertical distribution of absorbed PAR and NIR in the canopy are computed according to de Pury and Farquhar (1997). Potential evapotranspiration is based on ET_0 determined hourly using the FAO56 Penman-Monteith equation and adapted to soil cover through bare soil coefficient K_e and crop coefficient K_c (Allen et al., 1998; Allen et al., 2006).

Based on the resistance concept, the SVAT module interacts with FvCB and Leuning models to reach a value of stomatal conductance, and thus adjusts transpiration in line with the energy balance. Finally, the resulting crop transpiration is directly linked to the extraction of soil water by roots and can be limited because of edaphic stress (Hansen and Abrahamsen, 2009).

2.2.4. Input data and parameterisation

Hourly measurements of air temperature, global radiation, relative humidity, wind velocity and precipitation were collected from data measured at BE-Lon and used as

forcing data for Daisy. Additionally, measurements of water table depth were also provided as inputs to Daisy. For each growing season, input factors (i.e., forcing data and parameters) were gathered into a Daisy setup file. All parameters included in this GSA were explicitly defined in these files and set to their measured or default value. Input and setup files used for running Daisy are available in the supplementary material. Although the soil profile at BE-Lon is composed of three horizons, when soil texture, humus and dry bulk density were measured, the first horizon was distinguished into two soil layers resulting in four parameterised soil layers Table 3.2¹.

Table 3.2: Soil texture, humus and bulk density depending on soil depth. Standard deviations are indicated in parentheses.

Horizon	Depth (cm)	Clay (%)	Silt (%)	Fine sand (%)	Coarse sand (%)	Humus (%)	Bulk density (g cm ⁻³)
Ap1	0-15	11.4 (± 0.9)	78.7 (± 4.9)	5.8 (± 3.8)	2.3 (± 1.2)	1.9 (± 0.094)	1.23 (± 0.1)
Ap2	15-30	10.6 (± 0.8)	79.2 (± 4.9)	5.9 (± 3.8)	2.4 (± 1.2)	1.8 (± 0.11)	1.39 (± 0.05)
E or B	30-60	16.6 (± 1.3)	76.2 (± 4.6)	5.5 (± 3.8)	1.0 (± 1.0)	0.7 (± 0.11)	1.50 (± 0.02)
Bt	60-150	19.6 (± 1.5)	74.5 (± 4.4)	5.0 (± 3.7)	0.6 (± 1.0)	0.3 (± 0.077)	1.54 (± 0.03)

In order to initialise the content of the OM pools, a 10-year warm-up period was applied with typical field management and representative weather conditions. This period aims to assess the amount of carbon added to the organic matter system each year. With this information, repartition between OM pools could be estimated from quasi-equilibrium equations already implemented in Daisy (Hansen et al., 2012)².

2.3. Global sensitivity analysis

2.3.1. Parameter ranges and model outputs

In total, 200 parameters, involved in most processes simulated by Daisy, were considered for the screening step. These include parameters related to SOM decomposition, soil hydraulic dynamics, crop development and photosynthesis, energy balance, radiation and water distribution, soil nitrogen dynamics and anthropogenic nitrogen input. Only model parameters were considered in this analysis, even though GSA methods can be applied to all input factors, including weather and groundwater level data. Taking time series of forcing inputs into account is a complex task which is not covered in this paper, however, information can be found in Section 4.3 of Pianosi et al. (2016).

Uniform parameter distribution was assigned to all parameters and required explicit bounds. For each parameter, these bounds were determined according to site data,

¹Addendum: additional soil information are available at the end of this chapter (Tables 3.6 and 3.7).

²Addendum: the initial repartition was thus identical for each growing season, but residues from the previous crop was specified and incorporated as AOM.

literature or, if there was no information or physical meaning for a parameter, 20% variation either side of its reference value (López-Cruz et al., 2012; Casadebaig et al., 2016; Pianosi et al., 2016; Jabloun et al., 2018). All parameters, along with their reference value and bounds, are listed in the supplementary materials (Table 3.4).

Aiming to quantify and understand the influence of Daisy parameters on crop yield, GHG and energy fluxes, multiple outputs were considered in this analysis: (1) dry matter of storage organs (WSOrg), (2) NEE, (3) LE, (4) H and (5) nitrous oxide estimated with eq. (3.1) N_2O .

The Morris screening method is fully described in the supplementary materials, with associated results (Table 3.5). Parameters were selected for Sobol' analysis if they were among the 25 most influential parameters for at least one output.

2.3.2. Sobol' variance-based method

Variance-based methods aim to decompose the output variance of a model into relative contributions from each parameter and its interactions, considering output variance as a good proxy for output uncertainty (Pianosi et al., 2016; Van Werkhoven et al., 2008). The direct contribution of an individual parameter, called first-order sensitivity index, is computed as follows:

$$S_i = \frac{V[E(y | x_i)]}{V(y)} \quad (3.2)$$

where $V[E(y | x_i)]$ represents the variance, taken over all possible values of x_i , of the mean of output y when all parameters but x_i are varying (Saltelli et al., 2010) and $V(y)$ is the total output variance. The first-order index, varying from 0 to 1, quantifies the direct effect of a parameter. In this study, a parameter is considered to be significant if $S_i > 0.01$ (Sarrazin et al., 2016). On the other hand, total-order sensitivity index measures the total contribution of an individual parameter, i.e., the direct contribution and its interactions with other parameters:

$$S_{Ti} = 1 - \frac{V[E(y | X_{\sim i})]}{V(y)} \quad (3.3)$$

where $V[E(y | X_{\sim i})]$ represents the variance, taken over all possible values of $X_{\sim i}$, of the mean of y when only x_i is varying. It depicts the first-order contribution of all parameters but x_i . Therefore, S_{Ti} represents the relative contribution of all terms including x_i , directly or not. These sensitivity indices were computed according to the sampling scheme proposed by Sobol' (2001) and Saltelli (2002), using a numerical integration with Monte Carlo method (Herman et al., 2013).

2.3.3. Application of Sobol' method

In this case study, variables of interest WSOrg, NEE, LE, H, estimated N_2O are not scalar but vector outputs. Hourly outputs were averaged within each week to generate weekly outputs for the temporal GSA – over daytime (9-16h) for NEE, LE and

H. Sobol' sensitivity indices were then computed at weekly and hourly temporal resolutions. The weekly evolution of sensitivity indices aimed to discuss the seasonal changes whereas the hourly evolution, restricted to one day, focused on dynamics within a day. Regarding the aggregated GSA, model outputs were aggregated in two ways; (i) cumulative over the entire crop season (Table 3.1), hereinafter referred to as CUM, and (ii) by computing the RMSE between modelled and observed data (referred to as RMSE).

2.4. Software and data

All flux and meteorological data for BE-Lon can be downloaded from the ICOS Data Portal (Heinesch et al., 2022; Dumont et al., 2023). Daisy is an open-source model developed by the Agrohydrology group at the University of Copenhagen, Denmark (Hansen et al., 2012). In this application, version 6.33 of Daisy, implemented in C++, was called from Python scripts using the PyDaisy library and GSA calculations were then completed in Python with the SALib library (Herman and Usher, 2017). In terms of computational demand, 14 070 and 118 784 parameter sets were respectively evaluated for Morris and Sobol' analysis, with each model run taking approximately 10 seconds. Parallel processing was implemented using 30 threads, reducing the computation time considerably.

3. Results

3.1. Environmental conditions and observed data

The SAH variety experienced peculiar environmental conditions in terms of water dynamics, with heavy rainfall during winter and thus high soil water content until May (Figure 3.1). In contrast, SKY had the driest conditions, as shown by the significant decrease of soil water content (SWC)³, small amount of precipitation and high values of vapour pressure deficit (VPD). SKY nevertheless had the higher crop yield (Figure 3.1c). TOB and SMA cropping seasons had no extreme events (without heavy rainfall nor lengthy periods of dry weather), but it should also be noted that TOB early growth was characterised by an autumn with low precipitation and soil water content, but the development of vegetation is slow during this period. On the other hand, SMA experienced atmospheric dryness around July, as depicted by high values of VPD and LE.

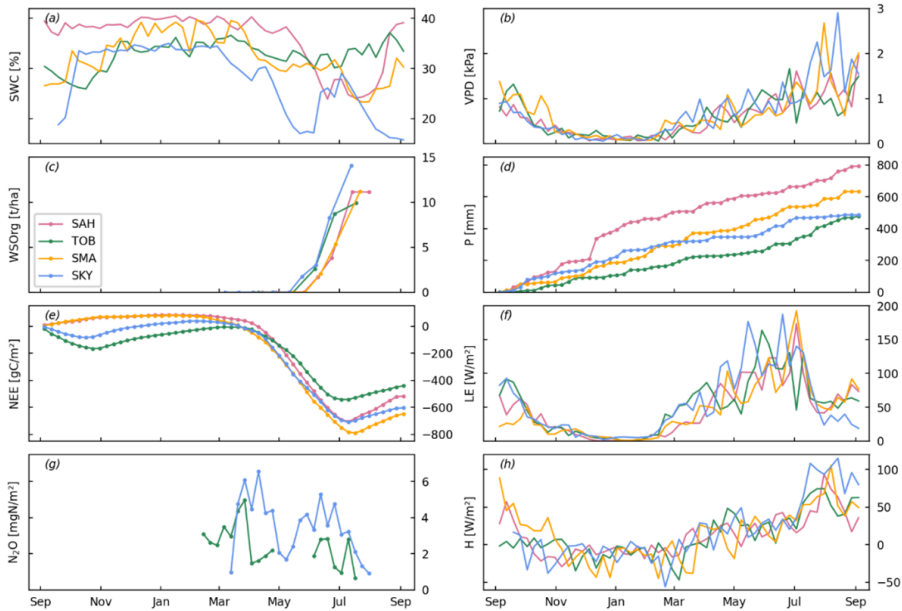


Figure 3.1: (a) SWC at 15 cm depth, (b) weekly mean of VPD, (c) WOrg, (d) annual cumulated precipitation (P), (e) annual cumulated NEE, (f) weekly mean of LE, (g) weekly cumulation of N₂O fluxes and (h) weekly mean of H fluxes for four winter wheat crops.

³Addendum: it is worth noting that SWC in winter greatly varies between seasons, which is likely due to changes in sensor type and their successive calibrations.

3.2. Aggregated global sensitivity analysis

Out of the 57 parameters selected with Morris screening (Table 3.5), 42 were found to significantly influence at least one output that was aggregated either with the CUM or RMSE objective function (Table 3.3).

Table 3.3: Description of influential parameters according to Sobol' aggregated analysis, ordered based on results of Morris screening.

Parameter	Units	Bounds	Description
fPSII	-	0.16–0.3	Fraction of PAR effectively absorbed by PSII
Xn	mol mol ⁻¹ s ⁻¹	0.0006–0.002	Ratio of photosynthetic capacity Vmax to leaf RubisCO-N
DO _{leun}	Pa	500–3500	Leuning empirical coefficient
c _{Vm}	-	25.5–29	Temperature scaling constant for Vmax
m _{leun}	-	9–18	Leuning stomatal slope
A _{brunt}	-	0.52–0.66	Brunt parameter (offset)
DSRate1	DS d ⁻¹	10%	Development rate during the vegetative stage
a	-	0.6–0.9	Atmospheric coefficient of shortwave radiation
σ _{NIR}	-	0.72–0.95	Leaf scattering coefficient of NIR
B _{brunt}	hPa ^{-0.5}	0.037–0.063	Brunt parameter (vapour pressure factor)
b _{leun}	mol m ⁻² s ⁻¹	0.008–0.02	Leuning stomatal intercept
k _{net}	-	0.35–0.5	Radiation extinction coefficient
NNI _{crit}	-	10%	Stem/leaf partitioning modifier (threshold)
f _{Leaf_{emg}}	-	10%	Leaf fraction of shoot assimilates at emergence
LfWidth	cm	2–5	Leaf width
volatilization	-	0.1–0.4	NH ₄ fraction that evaporates on application
LfDR _{fill}	d ⁻¹	20%	Leaf death rate during grain filling (DS=1.5)
Ksat _{aq}	cm h ⁻¹	0.01–0.05	Conductivity of the aquitard
LfDR _{anth}	d ⁻¹	20%	Leaf death rate at anthesis
PenPar2	°C	0–5	Root penetration rate parameter (threshold)
Ke	-	0.4–0.7	Conversion of ET ₀ to evaporation of bare soil
SpLAI	m ² gDM ⁻¹	0.016–0.02	Specific leaf area
ε _{leaf}	-	0.94–0.99	Leaf emissivity for long wave radiation
f _{RubisCO-N}	-	0.58–0.77	Fraction of leaf N as RubisCO-N
Z _{aq}	m	1–2.5	Thickness of the aquitard
ε _{soil}	-	0.91–0.97	Soil emissivity for longwave radiation
MxNH ₄ Up	g cm ⁻¹ h ⁻¹	1.13e-7–8.6e-7	Maximum NH ₄ uptake per unit root length
k _{SOM1}	h ⁻¹	6e-7–2e-6	Fraction of SOM1 converted to other pools (turnover rate)
PS _{NIR}	-	0.15–0.3	Soil reflection coefficient of NIR
f _{quartz}	-	2–10	Geometry factor for heat conductivity calculation
Ksat ₁	cm h ⁻¹	0.04–0.135	Hydraulic conductivity at saturation (1 st layer)
maintenance	h ⁻¹	4e-4–2e-3	Fraction used for staying alive (SMB2)
f _{absc}	-	0–0.7	Leaf abscission factor
F _{rel}	-	0.03–0.11	Fraction of max uptake accounted for by high affinity uptake
k _{10_{nit}}	gN cm ⁻³ h ⁻¹	1e-7–3e-7	Maximum rate (nitrification)
SRL	m g ⁻¹	100–200	Specific root length
r _{stem}	d ⁻¹	0.01–0.015	Maintenance respiration coefficient for stem
k _{nit}	gN cm ⁻³	3.2e-7–5e-5	Half saturation constant (nitrification)
ReMobilRt	d ⁻¹	0.01–0.04	Release rate of remobilization
ShldResC	%	20–50	Capacity of shielded reserves as fraction of WStem
ρ ₁	g cm ⁻³	1.03–1.43	Soil dry bulk density (1 st layer)
f _{nit}	-	0.008–0.02	Fraction of ammonium lost as N ₂ O

3.2.1. Objective function: CUM

Regarding crop yield (Figure 3.2), parameters displaying important first-order indices were photosynthetic parameters (Xn, c_{vm} , fPSII) as well as parameters related to the development of the vegetative stage DSRate1 and to the remobilisation of stem reserves (ReMobilRt and ShldResC). Energy fluxes (H and LE) are essentially influenced by Leuning and Brunt parameters, along with the conversion factor for bare soil evaporation Ke for LE and the leaf scattering coefficient of NIR σ_{NIR} and surface emissivity (ε_{soil} and ε_{leaf}) for H. Regarding the estimated N_2O , soil bulk density ρ_1 , nitrification parameters (f_{nit} and k_{nit}), photosynthetic parameters, uptake parameter MxNH4Up and SOM1 turnover rate k_{SOM1} were found to be influential. Finally, NEE was highly dependent on parameters related to photosynthesis.

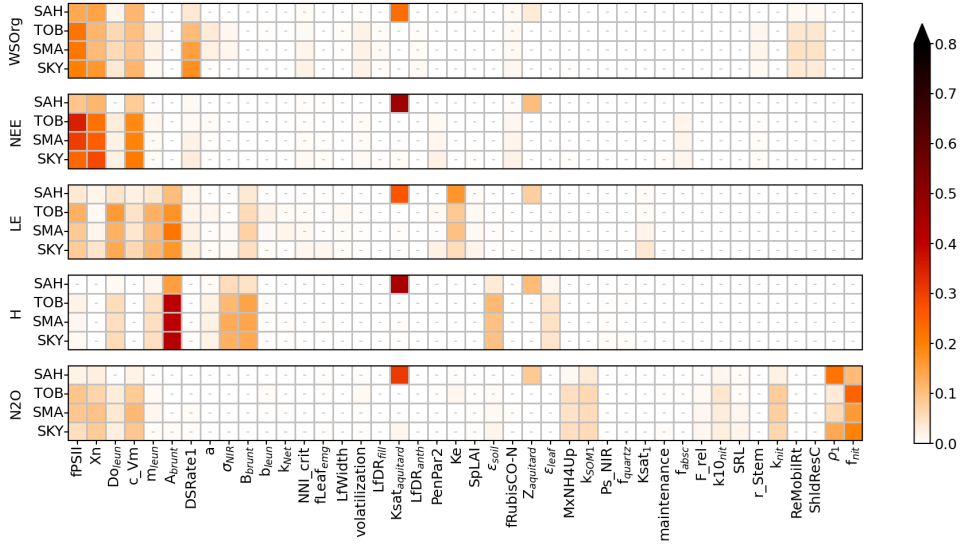


Figure 3.2: Sobol' first-order sensitivity indices S_i of significant parameters for all cumulative outputs (CUM) over each cropping season. Non-significant indices ($S_i < 0.01$) are labelled with a grey dash.

3.2.2. Objective function: RMSE

Although the most influential parameters for CUM (Figure 3.2) were also found to be significant for RMSE (Figure 3.3), many differences can be noted. For instance, Brunt parameters were no longer influential for LE, as was σ_{NIR} for H (Figure 3.3). Each cropping season has more contrasting results for RMSE; whereas only SAH stood out due to aquitard parameters for CUM (Figure 3.2), Figure 3.3 depicts this singularity along with others such as NEE greatly impacted by fPSII and Xn only for TOB.

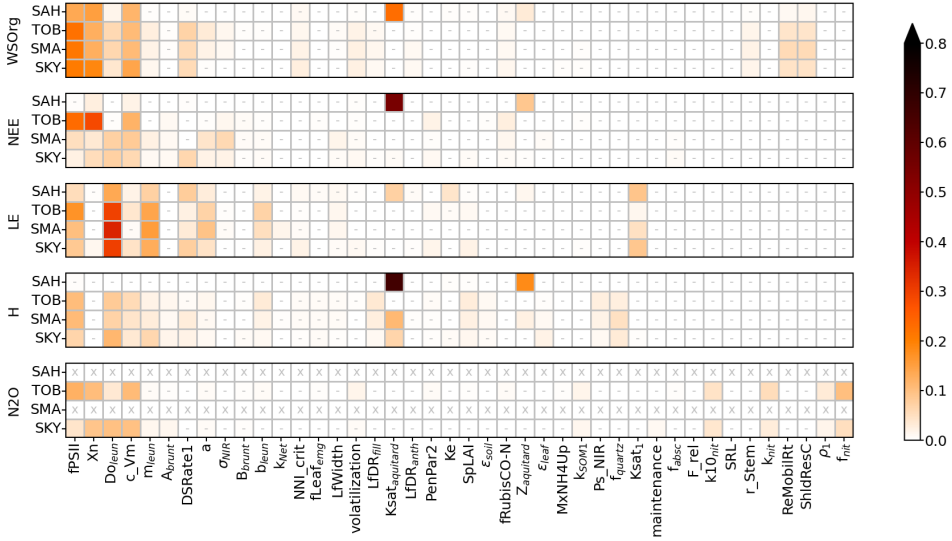


Figure 3.3: Sobol' first-order sensitivity indices S_i of significant parameters for all RMSE outputs over each cropping season. Non-significant indices ($S_i < 0.01$) are labelled with a grey dash. SAH and SMA are labelled with grey crosses because no measurements of N_2O fluxes were carried out, making the RMSE computation impossible.

3.2.3. Interactions between parameters

The first-order index S_i only expresses the direct contribution of a parameter to the output variance. However, parameters can also contribute to output variance through interactions between them. These interactions are computed as the difference between total-order and first-order indices ($ST_i - S_i$). Regarding the CUM outputs (Figure 3.2), a parameter's sensitivity essentially comes from its individual effect, as interactions are low (Figure 3.10). The interactions between some parameters are considerably higher when considering RMSE outputs (Figure 3.4).

Overall, interactions were especially high for parameters involved in photosynthesis, transpiration and energy balance, highlighting the complex interplay between these parameters. The SVAT module of Daisy interconnects the carbon and water cycle with the energy balance, as reflected by the importance of interactions among these parameters. The highest interaction is due to parameters Xn and C_{vm} as they both describe photosynthesis when the process is limited by Rubisco. When considering this interaction, TOB is no longer the only cropping season where photosynthetic parameters greatly impacted NEE.

Considering H fluxes, a large number of parameters had significant interactions. Brunt parameters and σ_{NIR} , which were highlighted in Figure 3.2 for H, were influential due to their interactions rather than their direct effect on RMSE. In addition to their

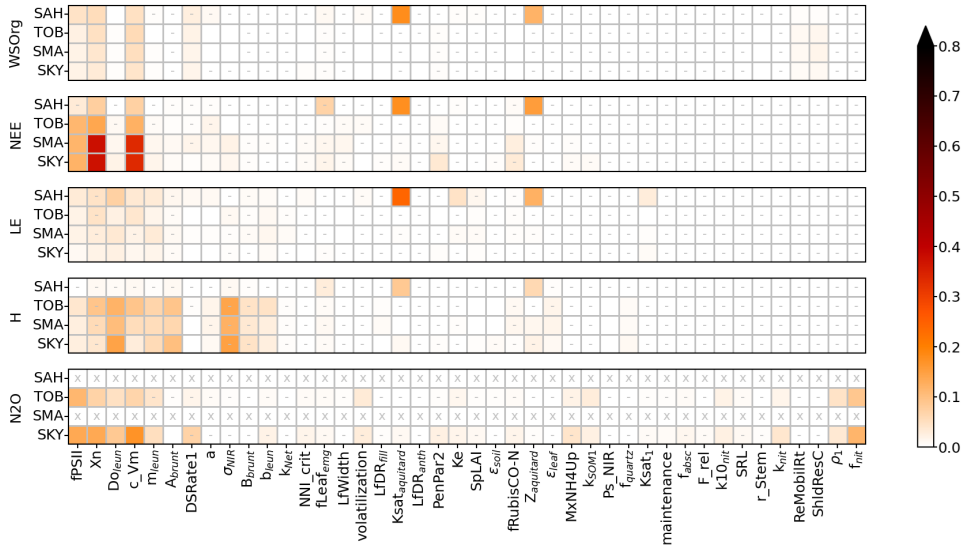


Figure 3.4: Sobol' interaction ($S_{Ti} - S_i$) of significant parameters for all RMSE outputs over each cropping season. Non-significant indices ($S_i < 0.01$) are labelled with a grey dash and impossible RMSE computations are labelled with grey crosses

mutual interactions, they also had high interactions with Leuning parameters. Whereas the first three parameters determine the energy absorbed by the system, Leuning parameters define the stomatal conductance that regulates the partitioning of this energy between H and LE. All these interactions underscore the importance of considering not only the individual effect of parameters but also their interactions in GSA and in future steps such as model calibration.

3.3. Temporal global sensitivity analysis

3.3.1. Net Ecosystem Exchange (NEE)

The weekly evolution of first-order indices depended upon vegetation development with clear changes around emergence, tillering and anthesis (Figure 3.5). In October, the crop has not yet emerged and the parameters involved in soil respiration (SOM turnover rate k_{SOM1} and maintenance of soil microbial biomass) were the most influential. The parameters contributing to the soil energy balance (A_{brunt} , B_{brunt} , ε_{soil}) also had a significant index, showing the dependence of soil respiration on soil temperature. From emergence to tillering (February), NEE was mainly influenced by the atmospheric coefficient a determining the diffuse and direct fraction of global radiation along with photosynthetic parameters (Xn , c_{vm} , f_{PSII}). At that time, the canopy was not dense, and the photosynthesis of the few developed leaves was tightly dependent on the composition (direct or diffuse) of global radiation. As vegetation was

developing, from February to late May, parameters related to photosynthetic processes became more influential.

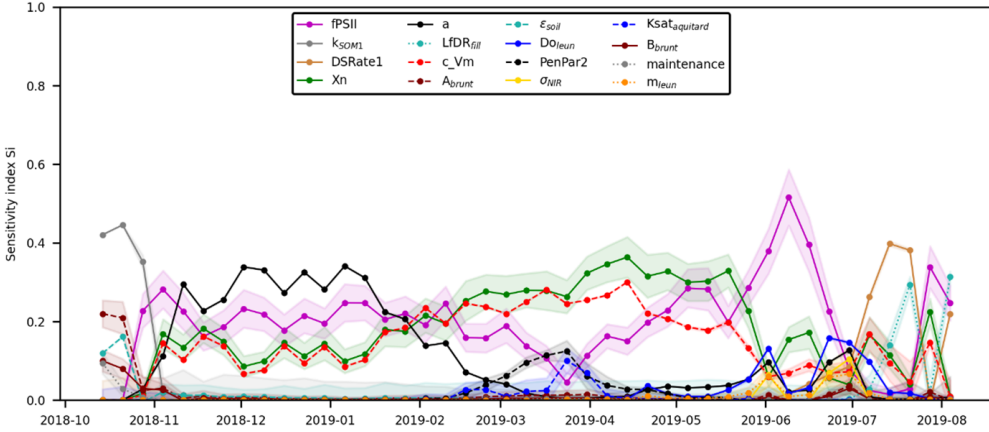


Figure 3.5: Weekly evolution of first-order sensitivity indices for NEE outputs (SMA). Parameters were depicted when S_i reached at least 0.05. Shaded areas correspond to standard deviations (*addendum: from Sobol' confidence intervals*), date indicates the 1st of each month.

Around March, the root penetration parameter PenPar2 gained influence as spring regrowth occurred, yet for a short time. As this parameter controls the rooting depth, it can limit the crop nitrogen uptake and thus carbon assimilation. Its influence increased along with vegetation and crop N requirement until the end of March. Around that time, N fertilisers were applied to the crop, leading to a decrease in PenPar2 influence. June, after anthesis, was the beginning of the reproductive stage, also known as the grain filling period. Consequently, photosynthetic parameters began to lose influence whereas DSRate1, which defines the start of the reproductive stage, gained influence along with the leaf death rate LfDR_{fill} that results in a decrease of carbon assimilation.

Hourly evolution of S_i was also found to be dynamic throughout a day (Figure 3.6). Photosynthetic parameters displayed opposite patterns with fPSII gaining influence near sunrise and sunset, whereas Xn and c_{Vm} had higher influence during daytime. This dual phenomenon is specific to the biochemical FvCB model, as carbon assimilation is either limited by RuBP generation (thus by light) or by Rubisco availability (thus by $V_{c,max}$). Around noon, in light-saturated conditions, carbon assimilation is mainly determined by $V_{c,max}$ which directly depends on Xn and c_{Vm} . On the other hand, in light-limited conditions (such as sunrise and sunset), fPSII is more important as it determines the amount of incident PAR utilised in electron transport for RuBP regeneration. This distinction between light-saturated and light-limited conditions can also be noticed in Figure 3.5, although it is less obvious. During winter, when global radiation was the lowest, fPSII was the most influential photosynthetic parameter while

NEE was highly influenced by X_n and c_{Vm} in spring, as conditions approached light saturation.

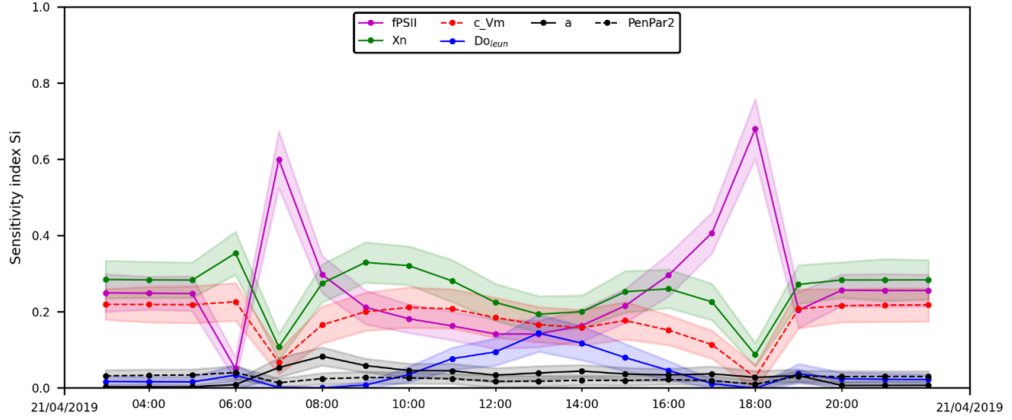


Figure 3.6: Hourly evolution of first-order sensitivity indices for NEE outputs (SMA) during a sunny day around stem elongation. Parameters were depicted when S_i reached at least 0.05. Shaded areas correspond to standard deviations.

The parameter related to stomatal conductance (Do_{Leun}) was also important during the day, suggesting a significant influence of stomatal conductance when solar radiation was high and when plants could open their stomata to increase CO_2 uptake. During night, $fPSII$, X_n and c_{Vm} were surprisingly the most important parameters for NEE even though there was no photosynthesis, but only soil heterotrophic respiration and plant autotrophic respiration. Considering the heterotrophic component, turnover rate of SOM pools would be expected to be influential. However, the period depicted in Figure 3.6 was characterised by significant growth and by a low amount of dead material. Therefore, heterotrophic respiration only accounted for about 10% of total respiration. Autotrophic respiration is dependent on accumulated crop dry matter, which is directly linked to the rate of photosynthesis. Photosynthetic parameters were thus also influential during night.

3.3.2. Energy fluxes (H & LE)

During winter, sensible heat fluxes were essentially controlled by the soil surface energy budget, as depicted by the influence of radiation parameters (A_{brunt} and B_{brunt}) and soil emissivity ϵ_{soil} (Figure 3.7). As the crop was growing and vegetation supplanted bare soil, H fluxes were no longer influenced by ϵ_{soil} but many crop parameters gained importance such as Leuning parameters (related to stomatal opening) and the leaf scattering coefficient for NIR σ_{NIR} . The two peaks of influence for $Ksat_{aq}$ and Z_{aq} correspond to periods of significant rainfall.

Similar evolutions can be observed with LE fluxes. When leaf coverage was low,

K_e (conversion factor from ET_0 to bare soil evaporation) and Brunt parameters had a significant impact on LE. While the crop was growing, these parameters began to lose their influence. After the tillering stage, the output variance was assigned to several crop parameters (some related to the stomatal conductance, to photosynthesis and to the water interception capacity IntcpCap), before being attributed to DSRate1 and Ksat1 during the reproductive stage.

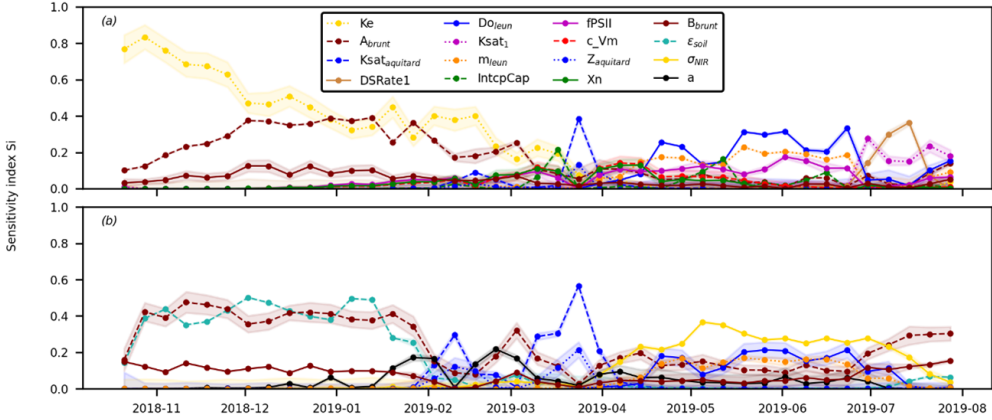


Figure 3.7: Weekly evolution of first-order sensitivity indices for (a) LE and (b) H outputs (SMA). Parameters were depicted when S_i reached at least 0.1. Shaded areas correspond to standard deviations, date indicates the 1st of each month.

As many parameters are concomitantly expressed after the tillering stage, Figure 3.8 provides a focus on a sunny day with the hourly evolution of S_i for both H and LE. On this day, H was composed of leaf sensible heat (66%) and soil sensible heat (33%) fluxes and LE was due to crop transpiration (80%) and soil evaporation (20%).

During daytime, parameters related to stomatal conductance and, to a lesser extent, photosynthesis became influential when solar radiation began to reach the vegetation, whether it be for H or LE. Stomatal aperture allows the plant to take up CO_2 but is always accompanied by a loss of water vapour, making transpiration tightly related to crop photosynthesis through stomatal conductance. As stomatal aperture controls LE fluxes, it also plays a key role in leaf energy balance. For higher stomatal conductance, a greater part of absorbed energy would be released as latent heat at the expense of sensible heat and canopy temperature would thus be lower.

Besides photosynthetic and stomatal parameters, the leaf scattering coefficient for NIR σ_{NIR} , extinction coefficient k_{net} and atmospheric coefficient a were also important during daytime. The first two parameters influence the radiation reaching the canopy and the soil surface, while a determines the diffuse fraction of radiation. Even if their impact is valid throughout the day, these parameters were more influential during sunrise, specifically for LE. It should be recalled that the sensitivity index S_i represents

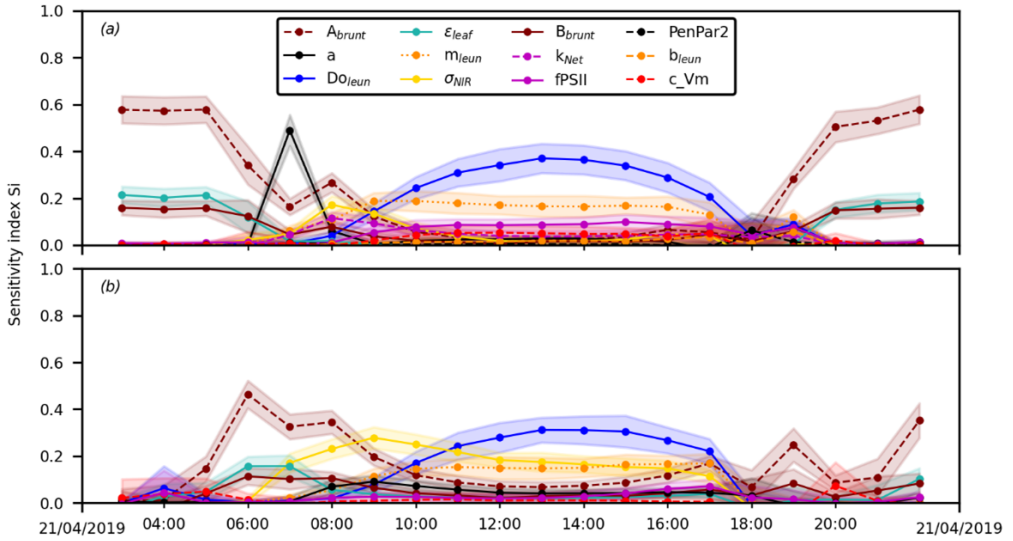


Figure 3.8: Hourly evolution of first-order sensitivity indices for (a) LE and (b) H outputs (SMA). Parameters were depicted when S_i reached at least 0.05. Shaded areas correspond to standard deviations.

the relative contribution of each parameter. Therefore, their indices are expected to decrease during the day as carbon assimilation takes place and stomatal and photosynthetic parameters gain influence at their expense.

During the night, only longwave radiation is absorbed by the soil and vegetation. This energy is then dissipated through latent and sensible heat. The variances of H and LE are thus mainly explained by Brunt parameters and leaf emissivity ϵ_{leaf} .

3.3.3. Estimated N_2O fluxes

Throughout the growing season, many parameters influenced the estimated N_2O fluxes, with a clear shift near tillering stage (Feb-Mar; Figure 3.9). During winter, dry bulk density of the first soil layer ρ_1 , soil emissivity ϵ_{soil} , Brunt parameter A_{brunt} , nitrification parameter f_{nit} and slow SOM turnover k_{SOM1} had a great impact on the estimated N_2O . ρ_1 defines the water-filled pore space, impacting the ratio of N_2O produced during denitrification. ϵ_{soil} and A_{brunt} are important for soil energy balance (see Figure 3.7b), hence for temperature conditions impacting denitrification and nitrification rates.

After February, photosynthetic parameters (c_{Vm} , X_n and $fPSII$), the parameter related to nitrogen uptake $MxNH4Up$ and nitrification parameters (k_{nit} , $k_{10_{nit}}$ and f_{nit}) gained influence. A major part of N_2O production seemed to come from nitrification, as shown by the half saturation constant k_{nit} and the maximum rate $k_{10_{nit}}$. During spring, their influence increased three separate times, precisely when farmers applied

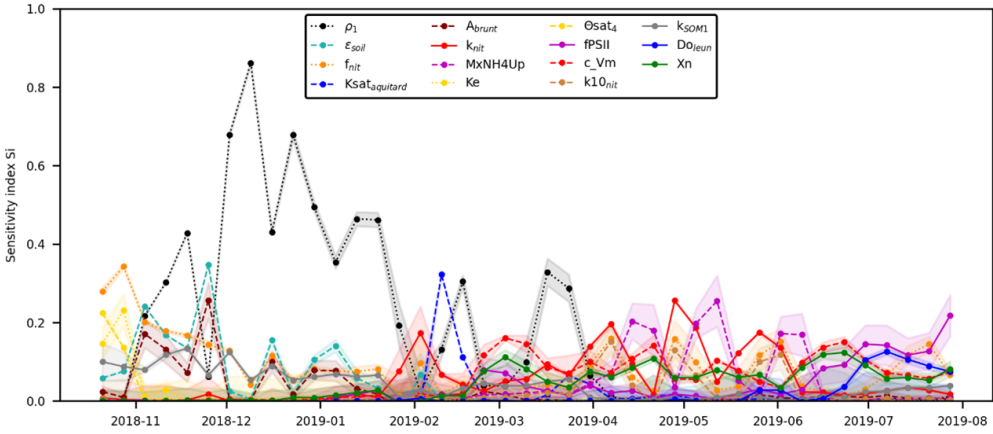


Figure 3.9: Weekly evolution of first-order sensitivity indices for the estimated N_2O outputs (SMA). Parameters were depicted when S_i reached at least 0.1. Shaded areas correspond to standard deviations, date indicates the 1st of each month.

fertilisers (on 25/03, 17/04 and 20/05), adding nitrates and ammonium into the soil. Afterwards, $MxNH_4Up$ index also increased as more ammonium was available for crop nitrogen uptake. Regarding photosynthetic parameters, their influence could also be attributed to crop uptake. Crop biomass production is highly influenced by these parameters (Figure 3.6) and needs nitrogen to properly grow, leading to a decrease of nitrate and ammonium availability for denitrification and nitrification processes, thus reducing N_2O emissions.

4. Discussion

4.1. *Temporal vs. aggregated analysis*

Whereas the aggregated analysis provides a unique index for each parameter, the temporal analysis revealed that the parameter indices changed considerably over time, and particularly with crop development (Section 3.3). Wang et al. (2013) reached the same conclusions when performing temporal GSA on grain biomass simulated by the WOFOST model. Although time-dependent indices are more difficult to interpret, they offer richer insights into the dynamics of the model.

Foremost, the analysis of these temporal dynamics deepened our comprehension of simulated processes and model behaviour, as discussed throughout Section 3.3. A few examples are the opposite daily patterns of c_{vm} , X_n and f_{PSII} (Figure 3.6) that were attributed to the two photosynthetic limitations implemented in the FvCB model or the influence of root parameter PenPar2 due to nitrogen deficiency (Figure 3.5). While all these parameters were highlighted by the aggregated analysis, considering the indices dynamics facilitated the identification and understanding of the related processes.

Additionally, temporal analysis also provides valuable information for calibration choices and helps to prevent misguided efforts. When aiming to calibrate a parameter, modellers can select periods of time when this parameter has a great influence and conduct measurement campaigns accordingly. For instance, for NEE outputs, calibration of photosynthetic parameters should be focused on Feb-May. Similarly, the parameter α , though not significant in the CUM-aggregated analysis (Figure 3.2), should be prioritised if NEE is poorly simulated during winter (Figure 3.5). Regarding the estimated N_2O , the influence of nitrification parameters is mainly localised around fertiliser applications but significantly decreases afterwards, allowing us to clearly identify when field campaigns should be carried out. In terms of calibration objectives, the hourly indices for NEE (Figure 3.6) suggested that photosynthesis and respiration should not be calibrated in two separate steps, as both processes are influenced by photosynthetic parameters.

Furthermore, temporal analysis allows the correctness of model behaviour to be verified through parameter sensitivities rather than model outputs (Reusser and Zehe, 2011; Song et al., 2013). Examining indices dynamics can help to locate modelling errors, which was the case when analysing the daily evolution of H and LE (Figure 3.8). It was expected that, during nighttime, the energy absorbed would mainly be released as H fluxes and that LE fluxes would be impacted by b_{leun} . In this period, stomata are nearly closed, meaning that the stomatal conductance is close or equal to b_{leun} (Le-

uning, 1995). Nevertheless, this assumption was inconsistent with Figure 3.8, where b_{leun} is influential only during daytime. This discrepancy revealed an oversight in the implementation of the water conductance during nighttime conditions in Daisy. It is worth noting that this error has a limited impact on the simulation outputs as they are close to zero during these hours. However, because of these low values, this error might have gone unnoticed when comparing outputs and measurements.

Lastly, as noted by Pianosi and Wagener (2016), data aggregation can cover interesting local behaviours. For instance, LE outputs were occasionally impacted by the aquitard parameter $K_{sat_{aq}}$ and the water canopy interception parameter $IntcpCap$ due to rainfall events (Figure 3.7). These parameters, while not significant in the aggregated analysis (Figures 3.2 and 3.3), could be crucial during localised extreme events such as intense rainfall. This is particularly relevant given the increasing frequency and intensity of extreme events due to climate change, which will significantly impact agriculture (IPCC, 2022).

In contrast to the temporal analysis, aggregated analysis has the advantage of lower computational demand. Considering only the time taken for Sobol' analysis, aggregated analysis was 50 times faster than the temporal weekly one. However, this computational time is minor compared to the time required to run the model simulations and data compilation. Altogether, we suggest using temporal analysis, whether for model understanding or calibration to observed data.

4.2. Impact of objective function

Aggregated SA results are highly dependent on the choice of the objective function (Pianosi et al., 2016). Definition of objective functions and their interpretation for hydrological models are well documented (Krause et al., 2005; Shin et al., 2013). Van Werkhoven et al. (2008) used four objective functions, aiming to capture different aspects in terms of hydrology and resulting in distinct sensitivities. Using multiple objective functions aims to limit information loss from data aggregation, but too many functions could also complicate the interpretation of results. Regarding SA on crop models, many studies focused on cumulative variables (e.g., crop yield or evapotranspiration) rather than using performance metrics like RMSE (DeJonge et al., 2012; Vanuytrecht et al., 2014; Casadebaig et al., 2016; Corbeels et al., 2016; Manevski et al., 2016a; Jabloun et al., 2018). On the other hand, sensitivity studies on SVAT or land surface models used such metrics (Pianosi et al., 2017) or averaged fluxes (Petropoulos et al., 2013; Raj Deepak et al., 2024). However, when dealing with crop or SVAT models, the use of multiple objective functions (average, metrics, summation, etc.) for one output has not been investigated, to our knowledge. In this study, two objective functions (CUM and RMSE) were applied to each model output and should be interpreted differently.

When CUM is applied to WSOrg, it helps us determine which parameters affect the

crop yield at harvest and what changes could be made in order to improve it. When applied to NEE or N_2O , it reflects the capacity of the ecosystem to act as a GHG source or sink. All the parameters that significantly influence these cumulative outputs play a key role in studying agricultural GHG fluxes and assessing mitigation benefits from specific cropping practices. Finally, when applied to H and LE, it can give insight into the role of agricultural parcels in the energy balance of the Earth's surface. Imbalance of the surface energy budget is a direct cause of surface warming (Stephens et al., 2012).

The CUM function captures the magnitude of an output, whereas RMSE includes field data and quantifies how close an output is to observations. This objective function emphasises parameters that are able to introduce major deviations from measurements. When aiming to better understand the model and its mechanisms, performance metrics like RMSE are not recommended (Gupta and Razavi, 2018). Moreover, including observed data with an objective function could generate undesired effects in the results due to noisy data (Reusser and Zehe, 2011). Nonetheless, they can help to identify parameters requiring more attention during calibration, instead of parameters that have a great impact on the output variable itself. This is the difference between identifiability analysis (i.e., which parameters improve the model fit to observed data) and sensitivity analysis (i.e., which parameters have a greater influence on the model's dynamic input-state-output behaviour) (Gupta and Razavi, 2018). These two analyses have distinct objectives and can produce different results, as confirmed in this study. For example, H fluxes were mainly impacted by photosynthetic, Leuning and aquitard parameters when considering RMSE (Figure 3.3), despite its output magnitude (CUM) being influenced by Brunt parameters, σ_{NIR} and $\varepsilon_{\text{soil}}$ (Figure 3.2). This discrepancy is due to poor modelling of H fluxes when these parameters are influential, e.g., following rainfall events as shown by the influence of aquitard parameters.

4.3. Influential Daisy parameters and over-parameterisation

Out of the initial 200 parameters, the Morris screening identified 17 influential parameters for WSOrg, 148 for NEE, 35 for LE, 125 for H and 29 for the estimated N_2O . The large number of parameters influencing NEE and H fluxes may be attributed either to the thresholds chosen in this study (Sarrazin et al., 2016), or to the inherent complexity of the simulated processes. NEE combines photosynthesis with both autotrophic and heterotrophic respiration, while H fluxes result from the surface energy balance, integrating evapotranspiration, radiation distribution and scattering, and other processes (Plauborg et al., 2010). However, considering the results of Sobol' analysis, where only 17 and 18 out of 57 selected parameters were found to be influential for NEE and H, the first hypothesis (i.e., thresholds being too low) seems more plausible. Although our parameter selection is not affected by the chosen thresholds, further work is needed to determine these thresholds if Morris is to be used as the primary GSA method.

Jabloun et al. (2018) applied Morris screening to Daisy, focusing on crop yield among other outputs. Even though their analysis used a less complex version of Daisy – without the SVAT or FvCB modules – our findings align with theirs in identifying a few parameters influencing crop yield, mainly related to photosynthesis and phenology. Similar to our study, parameters related to N concentration in plant organs were non-influential. One notable difference is the influence of parameters related to the remobilisation of stem reserves (ReMobilRt and ShldResC). This remobilisation process contributes significantly to grain yield, with contributions ranging from 19% to 54% in various wheat cultivars (Ehdaie et al., 2008), a finding supported by other studies (Maydup et al., 2010; Zhang et al., 2017), justifying the influence of these parameters for our case study.

In Daisy, a relatively small number of parameters were found to be influential compared to the total number included in the model. This trend is consistent with other SA applied to Daisy, where a few parameters were highlighted as influential (Manevski et al., 2016a; Manevski et al., 2016b; Liang et al., 2020; Motarjemi et al., 2021), specifically 34 and 36 out of 124 for two different seasons studied by Jabloun et al. (2018). Beyond improving model understanding, SA also plays a critical role in reducing the number of parameters that need to be estimated (Nossent and Bauwens, 2012; Pianosi et al., 2016). With complex models, over-parameterisation can become a serious issue and lead to equifinality problems (i.e., where multiple parameter sets produce the same model outputs) (Franks et al., 1997). According to Confalonieri et al. (2012), over-parameterisation in SUCROS-type models is mainly due to the use of tables adjusting parameter values based on temperature or development stage. This also applies to Daisy, where parameters like assimilate partitioning, specific N concentration in plant organs, or organ death rates are dependent on crop development and are governed by piecewise linear function (PLF). Along with SA methods, these functions could be simplified with parameters having clear biological meaning to address over-parameterisation, as done by Stella et al. (2014) for WOFOST.

4.4. Impact of environmental conditions

When comparing cropping seasons, SAH stood out because of the significant influence of the conductivity of the aquitard $K_{sat,aq}$ and, to a lesser extent, of the thickness of the aquitard Z_{aq} . As a consequence of heavy rainfall during winter for SAH, the soil profile was mostly saturated, with a water table depth varying between 30 and 100 cm for at least two months (Dec-Jan). From February, there were periods of several weeks with no rainfall, allowing the soil profile to gradually dry up. Soil water dynamics were mainly controlled by the conductivity of the underlying soil layer $K_{sat,aq}$ and its thickness Z_{aq} . High conductivity would speed up the draining of the soil profile while low conductivity would delay it, lengthening the waterlogged period. Around March, when the spring regrowth occurred, the development of vegetation was limited if the soil profile was still saturated. Under these conditions, water uptake was limited (and

thus the nitrogen uptake) due to the lack of evaporative demand and this resulted in nitrogen stress and a decrease of CO_2 assimilation. This limitation of crop development can be quite severe depending on the length of the waterlogged period.

Apart from the aquitard parameters, the aggregated analysis also highlighted the influence of K_{sat_4} and anisotropy (Figures 3.3 and 3.4). The former is the saturated conductivity of the 4th layer, just above the aquitard, and the latter represents the ratio between horizontal and vertical saturated flow. These parameters also impact the water conditions of the soil profile and play a role in the length of the waterlogged period.

The SKY cropping season was also depicted as a particular year in Section 3.1, with droughts during spring and summer. It was thus expected that parameters describing soil hydraulics and stomatal conductance, which link the carbon and water cycles, would have an increased influence compared to SMA and TOB cropping seasons. Jabloun et al. (2018) observed that yield sensitivity to soil parameters increased under water-limited conditions, even without the SVAT module. However, this is not reflected in Figures 3.2 and 3.3. Several factors could explain the lack of contrast in our results. First, the drought during the 2021-2022 season (SKY) may not have been severe enough, despite periods of high temperature, atmospheric dryness and edaphic dryness (Beauclaire et al., 2024a). They estimated that the relative extractable water (REW) went under 0.2 multiple times, but there was no clear impact on sun-induced chlorophyll fluorescence (SIF) and gross primary productivity (GPP) measurements. Second, our application did not account for stomatal conductance regulation by chemical signalling (Ahmadi et al., 2009; Plauborg et al., 2010), which might lead to different parameter sensitivities under varying environmental conditions. Finally, Daisy's current drought response, where stomatal conductance is regulated by hydraulic and chemical signals, may need refinement. Non-stomatal limitations, such as diffusive limitation related to the mesophyll conductance, biochemical, and photochemical limitations, could also be incorporated (Grassi and Magnani, 2005; Brestic and Zivcak, 2013).

Biochemical limitation is linked to parameters X_n and c_{V_m} as they determine the maximum rate of carboxylation $V_{c,\text{max}}$. Many studies have reported drought impacts on $V_{c,\text{max}}$, though these effects vary across species (Gourlez De La Motte et al., 2020; Beauclaire et al., 2023; Fang et al., 2023; Yang et al., 2023). Similarly, photochemical limitation, related to light absorption by photosystem II, can be linked to f_{PSII} . In water-stressed conditions, reduction in maximum quantum yield of PSII, which determines f_{PSII} , decreases the electron transport rate (Maxwell and Johnson, 2000; Long and Bernacchi, 2003; Liu et al., 2012; Guan et al., 2015; Trueba et al., 2019; Sommer et al., 2023). The above-mentioned parameters (X_n , c_{V_m} and f_{PSII}), which are crucial for carboxylation and electron transport, greatly impact photosynthesis but are not currently responsive to environmental conditions in the model. Incorporating these regulatory mechanisms could improve Daisy's drought modelling and would require

thorough calibration with drought-specific data.

4.5. Towards parameter estimation

As pointed out by Wallach et al. (2018), parameter estimation can either rely on direct measurement from the underlying processes or adjust the system model to data, which is commonly referred to as calibration. The first approach is preferable, as parameters should be measurable independently of any model structure and have a physical, chemical and/or physiological meaning (Sinclair and Seligman, 2000). This preserves the interpretability and realism of crop models.

In this application, some influential parameters could easily be estimated from measurements instead of being calibrated. For instance, shortwave and longwave radiation (incoming and outgoing) are measured in BE-Lon, allowing the Brunt parameters to be estimated independently from the model structure of Daisy. Furthermore, observations of phenological stages are also carried out at ICOS stations and are crucial for estimating DSRate1 and DSRate2.

In addition, supplementary measurements could enhance ecosystem understanding and parameter identifiability (Luo et al., 2009). For instance, manual measurements of chlorophyll fluorescence, with a portable plant efficiency analyser (LICOR-6400XT in Beauclaire et al. (2024a); Handy PEA for Wu et al. (2023)), can determine the maximum quantum yield of PSII $\Phi_{\text{PSII,max}}$. Besides quantifying plant water stress, the influential parameter f_{PSII} can be estimated as it is expressed as the product $\alpha_l \cdot \Phi_{\text{PSII,max}} \cdot \beta$ where α_l is the leaf absorbance in the PAR and β is the fraction of absorbed light that reaches PSII (Long and Bernacchi, 2003).

This GSA also underlined the essential role of the aquitard layer and its related parameters when the water table depth rises into the root zone due to large amounts of precipitation or poor drainage. Although SA of crop models usually focuses on parameters characterising the ploughed layer (Varella et al., 2012) or only considers a homogeneous profile (DeJonge et al., 2012; Thorp et al., 2020), aquitard parameters can significantly impact model outputs depending on the site and meteorological conditions. They should therefore be carefully estimated, recognising that direct measurements could be time-consuming and resource-intensive given the layer depth.

When influential parameters have to be calibrated (as they have no clear meaning or direct measurements are too complicated), computational resources, model characteristics, and the complexity of parameter interactions should be considered alongside algorithm robustness (Kavetski et al., 2018). Firstly, as crop models like Daisy capture complex dynamics that are mainly nonlinear, linear regressions such as ordinary or weighted least squares are less suitable (Currit, 2002). Secondly, Section 3.2.3 demonstrated that interactions between various parameters were significant and should not be overlooked during calibration. Estimating these parameters sequentially could introduce bias, as adjusted parameters could influence the values of others. On the other

hand, simultaneous methods can handle interactions between parameters, exploring the parameters' spaces concurrently. Examples of these methods include Bayesian approaches (Vrugt, 2016), the shuffled complex evolution (SCE) algorithm (Duan et al., 1994) or particle swarm optimisation method (Wang et al., 2018a; Gad, 2022).

Calibrating an over-parameterised model is a challenging task as it can lead to overfitting (Whittaker et al., 2010). As discussed in Section 4.3, GSA and model simplification can reduce the model over-parameterisation, and thus the risk of overfitting, by reducing the number of parameters considered for calibration. Moreover, temporal GSA can also provide critical guidance by identifying periods when specific parameters have the greatest influence. By focusing on these key periods, modellers can avoid overfitting parameters to less critical times and improve the efficiency of the calibration process. Finally, overfitting can also be limited by considering multiple target outputs during calibration (Gupta et al., 2003) or cross validation (Dinh and Aires, 2022; Yates et al., 2023).

5. Conclusion

This study demonstrates the complementary roles of temporal and aggregated GSA in characterising parameter influence within the Daisy crop model. While both approaches identified similar key parameters, temporal GSA highlighted dynamic shifts in sensitivity, emphasising critical periods for model calibration. These results underscore the potential of temporal GSA to improve the understanding of model structure and behaviour by capturing parameter effects that vary with temporal resolution. Beyond model understanding, temporal GSA also helped us to identify a small error in Daisy code that would have gone unnoticed otherwise, proving that this application may provide multiple benefits to model users.

Exploring objective functions in aggregated GSA revealed the dependence of sensitivity results on function choice. The cumulative (CUM) function effectively identified parameters impacting crop yield, CO₂, N₂O and energy fluxes, highlighting their roles in different environmental conditions. In contrast, the RMSE function, which incorporates measured data, identified parameters responsible for deviations from observations. This function aids model calibration by pinpointing influential parameters that affect model accuracy rather than output magnitude. This finding illustrates the value of combining diverse objective functions, depending on the user's objectives. In this study, the CUM function is informative for understanding system impacts and the RMSE function enhances model identifiability and calibration reliability.

Finally, the study highlights that, out of an initial 200 parameters, only a small subset was found to significantly influence outputs, underscoring the potential for model simplification in Daisy. By refining parameterisation through GSA, future studies can reduce model complexity while preserving accuracy.

6. Supplementary materials

Table 3.4: Description of all considered parameters with reference value and bounds. Values indicated by * depend on each cropping season, by ^a are based on measurements, by ^b are based on literature and by ^c correspond to largest feasible variation (<20% but without model failures nor impossible allocation dynamics)

Parameter	Units	Value ($\pm\sigma$)	Bounds or variation	Description
α_1	cm ⁻¹	0.00571 ($\pm 2.6\text{e-}4$)	$2\sigma^a$	Van Genuchten form parameter (1 st layer)
α_2	cm ⁻¹	0.0042 ($\pm 1.3\text{e-}4$)	$2\sigma^a$	Van Genuchten form parameter (2 nd layer)
α_3	cm ⁻¹	0.00515 ($\pm 1.8\text{e-}4$)	$2\sigma^a$	Van Genuchten form parameter (3 rd layer)
α_4	cm ⁻¹	0.00317 ($\pm 1.1\text{e-}4$)	$2\sigma^a$	Van Genuchten form parameter (4 th layer)
n_1	-	1.324 (± 0.02)	$2\sigma^a$	Van Genuchten parameter (1 st layer)
n_2	-	1.318 (± 0.013)	$2\sigma^a$	Van Genuchten parameter (2 nd layer)
n_3	-	1.267 (± 0.012)	$2\sigma^a$	Van Genuchten parameter (3 rd layer)
n_4	-	1.278 (± 0.034)	$2\sigma^a$	Van Genuchten parameter (4 th layer)
θ_{sat_1}	%	48.5	45–52.7 ^a	Soil water content at saturation (1 st layer)
θ_{sat_2}	%	46.5	42.7–50.7 ^a	Soil water content at saturation (2 nd layer)
θ_{sat_3}	%	42.3	40.7–43.8 ^a	Soil water content at saturation (3 rd layer)
θ_{sat_4}	%	40.7	38.5–43.1 ^a	Soil water content at saturation (4 th layer)
K_{sat_1}	cm h ⁻¹	0.112	0.04–0.135 ^a	Hydraulic conductivity at saturation (1 st layer)
K_{sat_2}	cm h ⁻¹	0.0704	0.04–0.081 ^a	Hydraulic conductivity at saturation (2 nd layer)
K_{sat_3}	cm h ⁻¹	0.109	0.04–0.129 ^a	Hydraulic conductivity at saturation (3 rd layer)
K_{sat_4}	cm h ⁻¹	0.0177	0.013–0.022 ^a	Hydraulic conductivity at saturation (4 th layer)
CperN_1	gC gN ⁻¹	10.0 (± 0.28)	$2\sigma^a$	Total carbon/nitrogen ratio (1 st layer)
CperN_2	gC gN ⁻¹	10.0 (± 0.30)	$2\sigma^a$	Total carbon/nitrogen ratio (2 nd layer)
CperN_3	gC gN ⁻¹	8.45 (± 0.46)	$2\sigma^a$	Total carbon/nitrogen ratio (3 rd layer)
CperN_4	gC gN ⁻¹	7.17 (± 0.86)	$2\sigma^a$	Total carbon/nitrogen ratio (4 th layer)
ρ_1	g cm ⁻³	1.23 (± 0.10)	$2\sigma^a$	Soil dry bulk density (1 st layer)

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Table 3.4: (continued)

Parameter	Units	Value ($\pm\sigma$)	Bounds or variation	Description
ρ_2	g cm^{-3}	1.39 (± 0.05)	$2\sigma^a$	Soil dry bulk density (2 nd layer)
ρ_3	g cm^{-3}	1.50 (± 0.02)	$2\sigma^a$	Soil dry bulk density (3 rd layer)
ρ_4	g cm^{-3}	1.54 (± 0.03)	$2\sigma^a$	Soil dry bulk density (4 th layer)
humus ₁	%	1.8 (± 0.094)	$2\sigma^a$	Soil humus fraction (1 st layer)
humus ₂	%	1.9 (± 0.11)	$2\sigma^a$	Soil humus fraction (2 nd layer)
humus ₃	%	0.7 (± 0.11)	$2\sigma^a$	Soil humus fraction (3 rd layer)
humus ₄	%	0.3 (± 0.077)	$2\sigma^a$	Soil humus fraction (4 th layer)
anisotropy	-	1	0.5–2.5 ^b	Ratio of horizontal Ksat to vertical Ksat
rpore _{min}	μm	0.1	20%	Size of smallest pores in the soil
CEC	cmolc kg^{-1}	12	5–25 ^b	Cation Exchange Capacity
b _{tort}	-	2	1–2.5 ^b	Theta factor for soil tortuosity
f _{quartz}	-	2	2–10 ^b	Geometry factor for heat conductivity calculation
f _{mineral}	-	4	2–10 ^b	Geometry factor for heat conductivity calculation
f _{nit}	-	0.02	0.008–0.02 ^b	Fraction of ammonium lost as N ₂ O
k _{nit}	gN cm^{-3}	5e-5	3.2e-7–5e-5 ^b	Half saturation constant (nitrification)
k10 _{nit}	$\text{gN cm}^{-3} \text{ h}^{-1}$	2.08e-7	1e-7–3e-7 ^b	Maximum rate (nitrification)
K _{denit}	h^{-1}	2.08e-2	20%	Maximum fraction of nitrate converted at each time step from slow pools
α_{denit}	$\text{gNO}_3\text{N gCO}_2\text{C}^{-1}$	0.1	20%	Anaerobic denitrification constant for slow pools
Ke	-	0.6	0.4–0.7 ^b	Conversion of ET ₀ to evaporation of bare soil
albedo _{dry}	-	0.15	0.14–0.2 ^b	Albedo of dry soil (pF >= 3)
albedo _{wet}	-	0.08	0.05–0.15 ^b	Albedo of wet soil (pF <= 1.7)
MaxRootDepth	cm	130	105–150 ^{a,b}	Depth at the end of the root zone
dispersivity	cm	5	0.5–6 ^b	Dispersion length
Ksat _{aq}	cm h^{-1}	0.01	0.01–0.05 ^{a,b}	Conductivity of the aquitard
Z _{aq}	m	2	1–2.5 ^b	Thickness of the aquitard
input	$\text{kgC ha}^{-1} \text{ y}^{-1}$	2906	20%	Amount of carbon added to the OM system

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Table 3.4: (continued)

Parameter	Units	Value ($\pm\sigma$)	Bounds or variation	Description
root	kgC ha ⁻¹ y ⁻¹	1355	20%	Amount of C added to the OM system from dead roots
end	cm	-30	-35-(-30) ^a	Depth of non-root input
maintenance	h ⁻¹	4.17e-4	4e-4-2e-3 ^b	Fraction used for staying alive (SMB2)
k _{SMB2}	h ⁻¹	4.17e-4	1e-4-6e-4 ^b	Fraction of SMB2 converted to other pools (turnover rate)
k _{SOM1}	h ⁻¹	1.79e-6	6e-7-2e-6 ^b	Fraction of SOM1 converted to other pools (turnover rate)
k _{SOM2}	h ⁻¹	5.83e-6	4.5e-6-1e-5 ^b	Fraction of SOM2 converted to other pools (turnover rate)
Z _{0b}	m	0.0006	0.0001-0.01 ^b	Bare soil roughness height for momentum
ε _{leaf}	-	0.98	0.94-0.99 ^b	Leaf emissivity for long wave radiation
ε _{soil}	-	0.95	0.91-0.97 ^b	Soil emissivity for longwave radiation
rb	s m ⁻¹	20	15-25 ^b	Boundary layer resistance for wet surface
a	-	0.84	0.6-0.9 ^b	Atmospheric coefficient of shortwave radiation
fa	-	0.5	0.4-0.5 ^b	Fraction of attenuated radiation reaching surface as diffuse
σ _{PAR}	-	0.15	0.12-0.18 ^b	Leaf scattering coefficient of PAR
σ _{NIR}	-	0.83	0.72-0.95 ^b	Leaf scattering coefficient of NIR
P _{SPAR}	-	0.1	0.08-0.2 ^b	Soil reflection coefficient of PAR
P _{SNIR}	-	0.18	0.15-0.3 ^b	Soil reflection coefficient of NIR
A _{brunt}	-	0.64	0.52-0.66 ^b	Brunt parameter (offset)
B _{brunt}	hPa ^{-0.5}	0.044	0.037-0.063 ^b	Brunt parameter (vapour pressure factor)
Xn	mol mol ⁻¹ s ⁻¹	0.00116	0.0006-0.002 ^b	Ratio of photosynthetic capacity Vmax to leaf RubisCO-N
Gamma25	Pa	3.69	3.6-4.2 ^b	CO2 compensation point of photosynthesis
Kc25	Pa	40.4	26-48.8 ^b	Michaelis-Menten constant of RuBisCO for CO2
Ko25	Pa	24800	16300-34300 ^b	Michaelis-Menten constant of RuBisCO for O2
c _{Vm}	-	26.35	25.5-29 ^b	Temperature scaling constant for Vmax
fPSII	-	0.28	0.16-0.3 ^{a,b}	Fraction of PAR effectively absorbed by PSII
kn	-	0.713	0.3-0.72 ^b	Extinction coefficient of nitrogen in the canopy
m _{leun}	-	11	9-18 ^b	Leuning stomatal slope
b _{leun}	mol m ⁻² s ⁻¹	0.01	0.008-0.02 ^b	Leuning stomatal intercept

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Table 3.4: (continued)

Parameter	Units	Value ($\pm\sigma$)	Bounds or variation	Description
Do_{leun}	Pa	1500	500–3500 ^b	Leuning empirical coefficient
δ_{leun}	MPa	0.7	0.4–1 ^b	Effect of crown water potential
volatilization	-	0.1	0.1–0.4 ^b	NH4 fraction that evaporates on application
N_{ferti}	kgN ha ⁻¹	-*	5% ^a	Amount of applied fertilisation
$EmrSMF_{sat}$	-	1	0.8–1 ^b	Soil moisture effect on emergence
$TSum$	°Cd	-*	10% ^a	Soil temperature sum at emergence
$DSRate1$	DS d ⁻¹	-*	10% ^a	Development rate during the vegetative stage
$DSRate2$	DS d ⁻¹	-*	10% ^a	Development rate during the reproductive stage
$SpLAI$	m ² gDM ⁻¹	0.0171	0.016–0.02 ^a	Specific leaf area
PAR_{ref}	-	0.06	0.03–0.1 ^b	PAR reflectance
k_{PAR}	-	0.6	0.45–0.7 ^b	PAR extinction coefficient
NIR_{ref}	-	0.51	0.35–0.55 ^b	NIR reflectance
k_{NIR}	-	0.18	0.18–0.28 ^b	NIR extinction coefficient
k_{net}	-	0.5	0.35–0.5 ^b	Radiation extinction coefficient
$IntcpCap$	mm	0.5	0.05–0.5 ^b	Interception capacity
Kc	-	1.2	1.1–1.3 ^b	Conversion of ET0 to crop evapotranspiration
PAR_{rel}	-	0.05	0.02–0.07 ^b	Relative PAR below the canopy
$LfWidth$	cm	3	2–5 ^b	Leaf width
H_1	cm	-*	5% ^a	Crop height at anthesis (DS=1)
$LAI_{Dist1z1}$	-	0.2	0.2–0.35 ^b	Relative CAI distribution density
$LAI_{Dist1z2}$	-	0.8	0.55–0.8 ^b	Relative CAI distribution density
$TaLim$	°C	5	20%	Vernalisation temperature threshold
$TaSum$	°Cd	-50	-55–(-45) ^b	Vernalisation temperature-sum requirement
DM_{frac}	%	87	85–90 ^{a,b}	Dry matter fraction in seeds
C_{frac}	%	45	39–45 ^{a,b}	Carbon fraction in seeds
N_{frac}	%	2	1.5–2.5 ^{a,b}	Nitrogen fraction in seeds
$rate_{seed}$	d ⁻¹	0.4	20%	Release rate of seed carbon to assimilate pool

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Table 3.4: (continued)

Parameter	Units	Value ($\pm\sigma$)	Bounds or variation	Description
fRubisCO-N	-	0.75	0.58–0.77 ^b	Fraction of leaf N as RubisCO-N
ShldResC	%	40	20–50 ^b	Capacity of shielded reserves as fraction of WStem
ReMobilDS	DS	1.1	1.1–1.2 ^b	Initial DS of remobilisation
ReMobilRt	d ⁻¹	0.03	0.01–0.04 ^b	Release rate of remobilization
CH2OReleaseRate	h ⁻¹	0.4	20%	CH2O release rate constant
E _{root}	gDM C g _{Ass} C ⁻¹	0.69	0.68–0.72 ^b	Conversion efficiency for root
E _{leaf}	gDM C g _{Ass} C ⁻¹	0.68	0.67–0.72 ^b	Conversion efficiency for leaf
E _{stem}	gDM C g _{Ass} C ⁻¹	0.66	0.65–0.69 ^b	Conversion efficiency for stem
E _{sorg}	gDM C g _{Ass} C ⁻¹	0.7	0.69–0.73 ^b	Conversion efficiency for storage organs
r _{root}	d ⁻¹	0.015	0.01–0.02 ^b	Maintenance respiration coefficient for root
r _{leaf}	d ⁻¹	0.016	0.01–0.03 ^b	Maintenance respiration coefficient for leaf
r _{stem}	d ⁻¹	0.01	0.01–0.015 ^b	Maintenance respiration coefficient for stem
r _{sorg}	d ⁻¹	0.01	0.01–0.02 ^b	Maintenance respiration coefficient for storage organs
f _{absc}	-	0.7	0–0.7 ^b	Leaf abscission factor
RtDR _{flag}	d ⁻¹	0.004	20%	Root death rate at flag leaf stage (DS=0.5)
RtDR _{anth}	d ⁻¹	0.02	20%	Root death rate at anthesis (DS=1)
RtDR _{mat}	d ⁻¹	0.03	20%	Root death rate at maturity (DS=2)
LfDR _{flag}	d ⁻¹	0.015	20%	Leaf death rate at flag leaf stage
LfDR _{anth}	d ⁻¹	0.027	20%	Leaf death rate at anthesis
LfDR _{fill}	d ⁻¹	0.065	20%	Leaf death rate during grain filling (DS=1.5)
LfDR _{mat}	d ⁻¹	0.08	20%	Leaf death rate at maturity
fRoot _{emg}	-	0.5	10% ^c	Root fraction of shoot assimilates at emergence (DS=0)
fRoot _{elong}	-	0.45	10% ^c	Root fraction of shoot assimilates at stem elongation (DS=0.3)
fRoot _{flag}	-	0.4	10% ^c	Root fraction of shoot assimilates at flag leaf stage
fRoot _{head}	-	0.16	10% ^c	Root fraction of shoot assimilates at heading (DS=0.8)

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Table 3.4: (continued)

Parameter	Units	Value ($\pm\sigma$)	Bounds or variation	Description
fRoot _{sflow}	-	0.04	10% ^c	Root fraction of shoot assimilates at the start of flowering (DS=0.95)
fLeaf _{emg}	-	0.72	10% ^c	Leaf fraction of shoot assimilates at emergence
fLeaf _{elong}	-	0.58	10% ^c	Leaf fraction of shoot assimilates at stem elongation
fLeaf _{flag}	-	0.53	10% ^c	Leaf fraction of shoot assimilates at flag leaf stage
fLeaf _{head}	-	0.3	10% ^c	Leaf fraction of shoot assimilates at heading
fLeaf _{sflow}	-	0.25	10% ^c	Leaf fraction of shoot assimilates at the start of flowering
fStem _{sflow}	-	0.62	10% ^c	Stem fraction of shoot assimilates at the start of flowering
fStem _{anth}	-	0.54	10% ^c	Stem fraction of shoot assimilates at anthesis
fStem _{eflow}	-	0.38	10% ^c	Stem fraction of shoot assimilates at the end of flowering (DS=1.1)
RSR _{anth}	-	0.5	20%	Maximum root/shoot ratio at anthesis
RSR _{mat}	-	0.25	20%	Maximum root/shoot ratio at maturity
NNI _{crit}	-	1.4	10% ^c	Stem/leaf partitioning modifier (threshold)
NNI _{inc}	-	0.65	10% ^c	Stem/leaf partitioning modifier (slope)
Rad	cm	0.015	0.01–0.022 ^{a,b}	Root radius
PenPar1	cm °C ⁻¹ d ⁻¹	0.25	0.1–0.25 ^b	Root penetration rate parameter (coefficient)
PenPar2	°C	4	0–5 ^b	Root penetration rate parameter (threshold)
MaxPen	cm	130	130–150 ^b	Maximum penetration length
MxNH4Up	g cm ⁻¹ h ⁻¹	2.5e-7	1.13e-7–8.6e-7 ^b	Maximum NH4 uptake per unit root length
MxNO3Up	g cm ⁻¹ h ⁻¹	2.5e-7	1.13e-7–8.6e-7 ^b	Maximum NO3 uptake per unit root length
Rxylem	-	10	20%	Transport resistance in xylem
SpRtLength	m g ⁻¹	152	100–200 ^{a,b}	Specific root length
DensRtTip	cm ⁻²	0.1	20%	Root length density at potential penetration depth
F _{relative}	-	0.1	0.03–0.11 ^b	Fraction of max uptake accounted for by high affinity uptake
K1	gN cm ⁻³	7e-7	5.1e-7–2.5e-6 ^b	K parameter for high affinity uptake
K2	gN cm ⁻³	7e-5	5.6e-5–1.5e-4 ^b	K parameter for low affinity uptake

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Table 3.4: (continued)

Parameter	Units	Value ($\pm\sigma$)	Bounds or variation	Description
PtLeafCnc _{till}	gN gDM ⁻¹	0.051	10% ^c	Upper limit for N conc. in leaves at tillering (DS=0.2)
PtLeafCnc _{flag}	gN gDM ⁻¹	0.048	10% ^c	Upper limit for N conc. in leaves at leaf flag stage
PtLeafCnc _{head}	gN gDM ⁻¹	0.044	10% ^c	Upper limit for N conc. in leaves at heading
PtLeafCnc _{anth}	gN gDM ⁻¹	0.038	10% ^c	Upper limit for N conc. in leaves at anthesis
PtLeafCnc _{mat}	gN gDM ⁻¹	0.021	10% ^c	Upper limit for N conc. in leaves at maturity
CrLeafCnc _{till}	gN gDM ⁻¹	0.039	10% ^c	Critical limit for N conc. in leaves at tillering
CrLeafCnc _{flag}	gN gDM ⁻¹	0.036	10% ^c	Critical limit for N conc. in leaves at leaf flag stage
CrLeafCnc _{anth}	gN gDM ⁻¹	0.025	10% ^c	Critical limit for N conc. in leaves at anthesis
CrLeafCnc _{mat}	gN gDM ⁻¹	0.014	10% ^c	Critical limit for N conc. in leaves at maturity
NfLeafCnc _{till}	gN gDM ⁻¹	0.01	10% ^c	Non-functional limit for N conc. in leaves at tillering
NfLeafCnc _{flag}	gN gDM ⁻¹	0.01	10% ^c	Non-functional limit for N conc. in leaves at leaf flag stage
NfLeafCnc _{anth}	gN gDM ⁻¹	0.006	10% ^c	Non-functional limit for N conc. in leaves at anthesis
NfLeafCnc _{mat}	gN gDM ⁻¹	0.005	10% ^c	Non-functional limit for N conc. in leaves at maturity
PtStemCnc _{till}	gN gDM ⁻¹	0.038	10% ^c	Upper limit for N conc. in stem at tillering
PtStemCnc _{flag}	gN gDM ⁻¹	0.035	10% ^c	Upper limit for N conc. in stem at leaf flag stage
PtStemCnc _{head}	gN gDM ⁻¹	0.02	10% ^c	Upper limit for N conc. in stem at heading
PtStemCnc _{anth}	gN gDM ⁻¹	0.015	10% ^c	Upper limit for N conc. in stem at anthesis
PtStemCnc _{mat}	gN gDM ⁻¹	0.011	10% ^c	Upper limit for N conc. in stem at maturity
CrStemCnc _{till}	gN gDM ⁻¹	0.023	10% ^c	Critical limit for N conc. in stem at tillering
CrStemCnc _{flag}	gN gDM ⁻¹	0.013	10% ^c	Critical limit for N conc. in stem at leaf flag stage
CrStemCnc _{head}	gN gDM ⁻¹	0.008	10% ^c	Critical limit for N conc. in stem at heading
CrStemCnc _{anth}	gN gDM ⁻¹	0.007	10% ^c	Critical limit for N conc. in stem at anthesis
CrStemCnc _{mat}	gN gDM ⁻¹	0.006	10% ^c	Critical limit for N conc. in stem at maturity
NfStemCnc _{till}	gN gDM ⁻¹	0.01	10% ^c	Non-functional limit for N conc. in stem at tillering
NfStemCnc _{anth}	gN gDM ⁻¹	0.002	10% ^c	Non-functional limit for N conc. in stem at anthesis
NfStemCnc _{mat}	gN gDM ⁻¹	0.002	10% ^c	Non-functional limit for N conc. in stem at maturity
PtSOrgCnc _{anth}	gN gDM ⁻¹	0.017	10% ^c	Upper limit for N conc. in storage organ at anthesis

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Table 3.4: (continued)

Parameter	Units	Value ($\pm\sigma$)	Bounds or variation	Description
PtSOrgCnc _{mat}	gN gDM ⁻¹	0.0175	10% ^c	Upper limit for N conc. in storage organ at maturity
CrSOrgCnc _{anth}	gN gDM ⁻¹	0.0125	10% ^c	Critical limit for N conc. in storage organ at anthesis
CrSOrgCnc _{mat}	gN gDM ⁻¹	0.0125	10% ^c	Critical limit for N conc. in storage organ at maturity
NfSOrgCnc _{anth}	gN gDM ⁻¹	0.0005	10% ^c	Non-functional limit for N conc. in storage organ at anthesis
NfSOrgCnc _{mat}	gN gDM ⁻¹	0.0005	10% ^c	Non-functional limit for N conc. in storage organ at maturity
PtRootCnc _{till}	gN gDM ⁻¹	0.025	10% ^c	Upper limit for N conc. in roots at tillering
PtRootCnc _{flag}	gN gDM ⁻¹	0.026	10% ^c	Upper limit for N conc. in roots at leaf flag stage
PtRootCnc _{head}	gN gDM ⁻¹	0.018	10% ^c	Upper limit for N conc. in roots at heading
PtRootCnc _{milk}	gN gDM ⁻¹	0.015	10% ^c	Upper limit for N conc. in roots at early milk (DS=1.2)
PtRootCnc _{mat}	gN gDM ⁻¹	0.014	10% ^c	Upper limit for N conc. in roots at maturity
CrRootCnc _{till}	gN gDM ⁻¹	0.017	10% ^c	Critical limit for N conc. in roots at tillering
CrRootCnc _{flag}	gN gDM ⁻¹	0.019	10% ^c	Critical limit for N conc. in roots at leaf flag stage
CrRootCnc _{head}	gN gDM ⁻¹	0.014	10% ^c	Critical limit for N conc. in roots at heading
CrRootCnc _{milk}	gN gDM ⁻¹	0.012	10% ^c	Critical limit for N conc. in roots at early milk
CrRootCnc _{mat}	gN gDM ⁻¹	0.009	10% ^c	Critical limit for N conc. in roots at maturity
NfRootCnc _{till}	gN gDM ⁻¹	0.009	10% ^c	Non-functional limit for N conc. in roots at tillering
NfRootCnc _{milk}	gN gDM ⁻¹	0.003	10% ^c	Non-functional limit for N conc. in roots at early milk
NfRootCnc _{mat}	gN gDM ⁻¹	0.003	10% ^c	Non-functional limit for N conc. in roots at maturity
TLLefEff	-	0.9	20%	Translocation efficiency (leaf)
TLRootEff	-	0.1	20%	Translocation efficiency (root)
EcoYield _W	-	0.85	0.82–0.88 ^a	Valuable fraction of storage organ (DM)
EcoYield _N	-	0.94	0.92–0.96 ^a	Valuable fraction of storage organ (N)

Morris screening method

The Morris screening method (Morris, 1991) is a computationally efficient GSA technique based on the One-At-a-Time (OAT) sampling design (Pianosi et al., 2016). This method allows to screen out non-influential from influential parameters and rank parameters in order of importance. Considering a model output $y(X)$ and a given set of parameters $X = (x_1, \dots, x_i, \dots, x_k)$, the elementary effect of the i -th parameter $d_i(X)$ is computed according to:

$$d_i(X) = \frac{y(x_1, \dots, x_i + \Delta, \dots, x_k) - y(X)}{\Delta} \quad (3.4)$$

where Δ is a predetermined multiple of $\frac{1}{p-1}$ with p equal to 8 (Pianosi et al., 2016). As suggested by Ruano et al. (2012), the number of trajectories in the parameter space was taken as 70. On all sampling possibilities, simulations leading to a model failure were spotted and a decision classification tree was used in order to identify the parameter combination causing this failure. Bounds of these parameters were restricted before restarting the simulations. The mean of the sampled elementary effects d_i , called μ_i , represents the influence of the i -th parameter on the output. As Daisy is a non-monotonic model, and thus elementary effects could cancel each other out, the influence of the i -th parameter was estimated with μ_i^* the mean of the absolute values of d_i (Campolongo et al., 2007).

Morris method was applied for each time step of Daisy outputs, resulting in time-dependent sensitivity indices $\mu_{i,t}^*$ (Song et al., 2013). The sensitivity index is relative to model outputs, expressed in the same units, and is thus case-specific (Sarrazin et al., 2016). To enable comparison between different outputs, a normalised sensitivity index was estimated as:

$$N_i = \frac{\sum_{t=0}^n \max(\mu_{i,t}^* - \mu_T^*; 0)}{\mu_T^*} \quad (3.5)$$

where μ_T^* is a threshold value, chosen as an acceptable variation of the concerned model output (Vanuytrecht et al., 2014). The threshold value was set to 0.3 t ha^{-1} for dry matter of storage organs WSOrg, 0.2 mm (around 5 W m^{-2}) for LE fluxes and 2 W m^{-2} for H fluxes (*addendum: based on the sensor detection/precision*). It was considered that a value above $0.25 \text{ gC m}^{-2} \text{ d}^{-1}$ and $0.25 \text{ mgN m}^{-2} \text{ d}^{-1}$ was significant for NEE and N_2O , which is based on (5% of) the daily mean (Suleau et al., 2011) and (50% of) the background emission (Lognoul et al., 2019). Finally, for each output, parameters were ranked according to the value of N_i . They were selected for Sobol' analysis if they were among the 25 most influential parameters for at least one output, they were otherwise set to their reference value.

Table 3.5: Morris ranking of the 57 selected parameters according to the normalised index N_i over all four growing seasons for each output. No sensitivity is denoted by "-".

Parameter	WSOrg	NEE	LE	H	N2O
fPSII	2	2	3	6	6
Xn	3	1	9	8	5
DO _{jeun}	6	5	1	3	-
CV _m	4	3	12	10	8
m _{jeun}	11	7	2	5	-
A _{brunt}	-	11	4	1	21
DSRate1	1	7	6	14	-
a	12	4	10	7	26
σ_{NIR}	16	10	15	2	-
B _{brunt}	-	21	14	4	-
b _{jeun}	-	19	10	12	-
SpLAI	-	13	19	13	-
NNI _{crit}	8	14	17	23	-
fLeaf _{emg}	-	9	30	17	-
LfWidth	-	17	18	22	-
volatilization	12	12	28	35	6
fRubisCO-N	-	6	-	25	-
Ksat _{aq}	14	30	16	21	12
LfDR _{fill}	9	25	20	24	-
PenPar2	-	15	-	33	16
Ke	-	54	5	20	19
k _{net}	-	48	8	16	-
ϵ_{soil}	-	43	-	9	-
σ_{PAR}	-	36	27	18	-
fRoot _{emg}	-	24	-	28	-
LfDR _{anth}	17	27	23	31	-
Z _{aq}	15	45	21	26	13
ϵ_{leaf}	-	50	24	11	-
fLeaf _{elong}	-	22	32	36	-
Kc25	-	16	-	43	-
PenPar1	-	18	-	50	29
Gamma25	-	19	-	55	-
MxNO3Up	-	23	-	58	-
k _{PAR}	-	28	24	54	-
MxNH4Up	-	29	-	63	3
Ksat ₄	-	56	35	32	17
ksOM1	-	25	-	62	10
P _{sNIR}	-	78	-	19	-
f _{quartz}	-	84	-	15	-
Ksat ₁	-	91	7	29	-
IntcpCap	-	73	13	52	15
maintenance	-	38	-	90	9
θ_{sat4}	-	76	-	44	23
f _{absc}	-	31	-	-	14
anisotropy	-	82	-	51	20
SRL	-	57	-	79	11
k10 _{nit}	-	67	-	88	3
F _{rel}	-	52	-	106	18
Ksat ₃	-	91	-	55	25
r _{stem}	9	58	-	98	-
Kc	-	97	22	53	-
k _{nit}	-	81	-	100	2
ReMobilRt	5	65	-	-	-
ShldResC	7	74	-	-	-
ρ_1	-	108	-	87	23
MaxRootDepth	-	103	-	116	22
f _{nit}	-	135	-	120	1

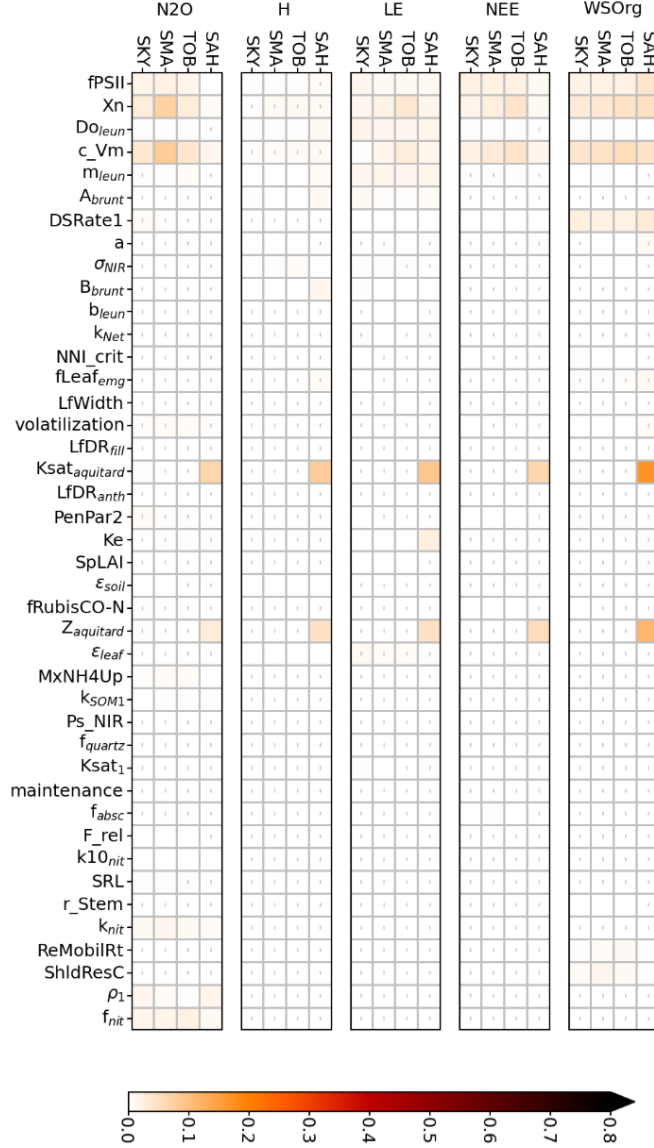


Figure 3.10: Sobol' interaction ($S_{Ti} - S_i$) of significant parameters for all CUM outputs over four cropping seasons. Non-significant indices ($S_i < 0.01$) are labelled with a grey dash and impossible RMSE computations are labelled with grey crosses.

7. Addendum

Table 3.6: Soil carbon and nitrogen characteristics measured in 2017. Standard deviations are indicated in parentheses.

Depth (cm)	CaCO ₃ (g/kg)	Corg (g/kg)	OM (g/kg)	N _{tot} (g/kg)	C/N
0-5	3.00 (± 1.33)	11.06 (± 0.72)	19.12 (± 1.23)	1.09 (± 0.06)	10.12 (± 0.29)
5-15	3.16 (± 1.38)	10.72 (± 0.55)	18.54 (± 0.94)	1.07 (± 0.05)	10.04 (± 0.28)
15-30	3.95 (± 1.70)	10.74 (± 0.63)	18.57 (± 1.07)	1.07 (± 0.06)	10.03 (± 0.30)
30-60	-	3.96 (± 0.66)	6.85 (± 1.14)	0.47 (± 0.06)	8.45 (± 0.46)
60-100	-	1.80 (± 0.44)	3.12 (± 0.77)	0.25 (± 0.04)	7.17 (± 0.86)

Table 3.7: Soil water properties measured in 2022 and fitted with LABROSSoilView-Analysis software. Soil water content at wilting point (WP) corresponds to $pF = 4.2$, and soil water contents at field capacity (FC) indicate $pF = 1.8$ and $pF = 2.5$.

Depth (cm)	θ_{sat} (%)	$\theta_{\text{FC},1.8}$ (%)	$\theta_{\text{FC},2.5}$ (%)	θ_{WP} (%)	K_{sat} (cm h ⁻¹)	L (-)
0-15	48.5	45.84	36.52	11.26	0.0274	-5.57
15-30	46.5	44.74	37.45	12.23	0.0216	-6
30-60	42.3	40.42	33.91	13.04	0.0333	-5.04
80-100	40.7	39.45	34.99	13.67	0.00946	-4.30

Interpreting carbon-water trade-offs in Daisy crop model using Pareto-based calibration

Preamble. Chapter 3 identified the most influential parameters of the Daisy–SVAT model and revealed how their influence evolves over the growing season. Building on this knowledge, Chapter 4 moves to the following steps of the modelling workflow, namely calibration and validation. This chapter tackles a challenge that is inherent to coupled carbon-water models: the objectives associated with different observed fluxes are often conflicting, so that improving the simulation of one tends to degrade another. Chapter 4 addresses this by applying a Pareto-based multi-objective calibration strategy, simultaneously targeting dry matter, NEE and LE for four winter wheat seasons at BE-Lon. This Pareto-based strategy identifies trade-offs between conflicting targets and hence can be used to highlight and interpret model structural limitations. In the following chapter, we explore an alternative photosynthesis representation, trying to alleviate some of the limitations reported here.

For this fourth chapter, I made amendments to the Daisy code, implemented the Pareto-based calibration method with the useful advice from Eric Laloy and wrote the manuscript. Eric Laloy also helped design the conceptual ideas and reviewed the manuscript. Quentin Beauclaire and Bernard Longdoz contributed to the interpretation of the results and also reviewed the manuscript. It has been published as:

Delhez, L., Laloy, E., Beauclaire, Q., and Longdoz, B.: Interpreting carbon-water trade-offs in Daisy crop model using Pareto-based calibration, *Biogeosciences*, 23, 2079–2099, <https://doi.org/10.5194/bg-23-2079-2026>, 2026.

Abstract. Improving the simulation of carbon and water exchanges is crucial for reliable crop modelling under changing climate conditions. Although model calibration is a key step, optimising multiple outputs can be challenging and often reveals trade-offs between calibration objectives. We applied a Pareto-based multi-objective calibration with the Speed-constrained Multi-objective Particle Swarm Optimisation (SMPSO) algorithm to the Daisy soil–plant–atmosphere model, targeting dry matter (DM), net ecosystem exchange (NEE), and latent heat flux (LE) of winter wheat crops. The optimal parameter set provided satisfactory results for all objectives (RMSE = 0.948 t ha⁻¹ for DM, 1.49 gC m⁻² d⁻¹ for daily NEE and 30.7 W m⁻² for daily LE) but revealed singular trade-offs. The strong compromise between dry matter and NEE likely suggests wrong parameterisation and/or measurement bias, while the trade-off between NEE and LE reflects equifinality issues from evapotranspiration partitioning. Lastly, this analysis also highlighted limitations in simulating stomatal regulation during heatwave conditions, supporting the decoupling between transpiration and carbon assimilation. These findings show that Pareto-based calibration can also serve as a diagnostic tool, identifying structural weaknesses and guiding targeted improvements in process representation for more robust crop model evaluation.

1. Introduction

Crop models are essential tools for yield forecasting and decision-making, but also for assessing the impact of climate change and understanding the complex interactions within the soil–plant–atmosphere continuum (Asseng et al., 2019). Over recent decades, they have been actively developed to account for changing environmental conditions such as rising temperature and elevated atmospheric CO₂ (Timlin et al., 2024). As a result, crop models now integrate more complex approaches and detailed processes, replacing, for instance, the tipping-bucket approach with Richard’s equation for soil water dynamics, or using biochemical photosynthesis models (Farquhar et al., 2001) instead of radiation-use efficiency. Biochemical models are often coupled with stomatal conductance models to jointly simulate CO₂ and water fluxes (Keenan et al., 2010). Such couplings are now implemented in advanced crop models such as GECROS (Yin and Van Laar, 2005) and Daisy (Plauborg et al., 2010), as well as in most terrestrial biosphere models (e.g., SiB2, ORCHIDEE, IBIS, JULES, etc.). These biosphere models have also been combined with crop models in order to improve crop development and yield predictions while accurately simulating gas exchanges. Some examples are SiBcrop (Lokupitiya et al., 2009), ORCHIDEE–STICS (De Noblet-Ducoudré et al., 2004), Agro–IBIS (Kucharik, 2003) and JULES–SUCROS (Van Den Hoof et al., 2011).

In these couplings, carbon and water fluxes between vegetation and atmosphere are assumed to only be regulated by stomatal behaviour. Widely used models of stomatal conductance g_s can be generally expressed as:

$$g_s = g_0 + g_1 \cdot f(E) \cdot A_{net} \quad (4.1)$$

where A_{net} is the net leaf CO₂ assimilation rate, $f(E)$ is a function of environmental influences such as vapour pressure deficit (VPD), g_0 and g_1 are parameters. When water is not limiting, plants open their stomata to maximise their carbon uptake. Conversely, they reduce their stomatal aperture under water stressed conditions, compromising between carbon assimilation and water loss (Manzoni et al., 2011). This response is often represented by a decrease of the slope parameter g_1 (Zhou et al., 2013; Liu et al., 2009). However, as stomatal behaviour is influenced by multiple drivers (soil water status, atmospheric dryness, leaf temperature, etc.) which often co-exist during extreme events such as droughts or heatwaves, plant responses may sometimes be contradictory (Grossiord et al., 2020). To date, these complex interactions remain poorly understood and insufficiently represented in models (Liu et al., 2024b; Sabot et al., 2022).

In this context, where stomatal behaviour controls both carbon assimilation and water loss, model calibration requires simultaneous assessment of different outputs. Calibrating against a single output (e.g., evapotranspiration) can result in compensating errors or masking structural deficiencies (Cameron et al., 2022). Multi-objective calibration therefore provides a well-suited framework, although it presents a significant challenge due to the high-dimensional parameter space of such models, the large computational cost of search algorithms and the potentially conflicting nature of targeted objectives. Extensively used in calibration of hydrological models (Efstratiadis and Koutsoyiannis, 2010; Jahandideh-Tehrani et al., 2020; Moges et al., 2020), multi-objective optimisation (MOO) algorithms aim to optimise all objectives simultaneously and explicitly handle conflicting objectives by exploring trade-offs using a Pareto-based sampling approach (Sharma and Kumar, 2022). This method allows modellers to select any points on the Pareto front, i.e., select an optimal parameter set depending on the modeller's preference (Tang et al., 2018).

Beyond identifying optimal parameter sets, Pareto-based calibration can also provide valuable insights into model behaviour. It can help detect ill-posed models, revealing structural inadequacies, missing processes, or equifinality (i.e., when multiple parameter sets provide similar results) (Kollat et al., 2012; Efstratiadis and Koutsoyiannis, 2010). Recently, Harvey et al. (2023) analysed the change of the Pareto front solutions between calibration and validation sets, revealing the influence of data type and model structure. Another study used Pareto-optimal solutions as informative prior distributions to guide posterior uncertainty estimation within a Bayesian framework (Tang et al., 2018).

In this case study, five growing seasons of winter wheat, cultivated on a Belgian site, were simulated using Daisy soil–plant–atmosphere model (Hansen et al., 2012). In addition to the stomatal coupling implemented with Farquhar biochemical model (Plauborg et al., 2010), this open-source model explicitly simulates the surface energy budget. Soil water movement is described by Richards' equation while accounting for drainage pipes, which are widely installed in agricultural fields. Together, these features make Daisy suitable for studying crop yield as well as coupled carbon and water flux dynamics under current and future conditions.

In a previous paper, we identified key parameters controlling crop yield, energy and carbon fluxes and discussed the implications of contrasting water conditions on sensitivity analysis results (Delhez et al., 2025). The objective of this follow-up study was twofold: to improve the simulation of biomass, carbon and water fluxes through calibration, and to explore the trade-offs between these outputs. To this end, we applied a swarm-based MOO algorithm called Speed-constrained Multi-objective Particle Swarm Optimisation (SMPSO) targeting dry matter of vegetation organs (DM), net CO₂ ecosystem exchange (NEE) and latent heat flux (LE). Accurate simulation of these variables is essential for food production assessments and for quantifying crop

carbon and water budgets. Furthermore, analysing trade-offs, particularly between carbon (NEE) and water (LE) fluxes, could reveal potential limitations in their coupled representation within the model¹.

¹Addendum: compared to Chapter 3, which also included N₂O and H, the number of targeted outputs was reduced in this chapter. Besides improving clarity, these two outputs were not considered because of, on the one hand, the lack of systematic measurement and established model representation for N₂O and, on the other hand, the similarity between influential parameters for both H and LE.

2. Materials and methods

2.1. Case study

The study site is a 12 ha cropland located in Lonzée, Belgium, with a temperate maritime climate ($\bar{T} = 11.1^{\circ}\text{C}$ and annual precipitation of 716 mm)². Cultivated for more than 85 years on a silt loam soil, this site has been equipped with an eddy covariance monitoring system and a micrometeorological station since 2004, as a part of the Fluxnet network. Since 2017, this monitoring site has integrated the ICOS network as a Level 2 station named BE-Lon.

This study focuses on five growing seasons of winter wheat (*Triticum aestivum* L.) which are summarised in Table 4.1³. Sown in late October, varieties from S17 and S22 are known to reach heading and maturity stages faster than Sahara and Smart cultivars (Meza et al., 2018; Meza et al., 2023). As the same cultivar was sown during S11 and S15, S11 was selected for the validation.

Table 4.1: Summary of winter wheat crops in BE-Lon. Coverage of NEE and LE corresponds to the fraction of high-quality hourly data during the calibration period.

	S11	S15	S17	S19	S22
Variety	Sahara	Sahara	Tobak	KWS Smart	LG Skyscraper
Sowing–Harvest	14 Oct 2010– 16 Aug 2011	14 Oct 2014– 2 Aug 2015	29 Oct 2016– 30 Jul 2017	10 Oct 2018– 1 Aug 2019	28 Oct 2021– 24 Jul 2022
Anthesis ($\pm 5\text{d}$)	10 Jun 2011	28 Jun 2015	15 Jun 2017	12 Jun 2019	9 Jun 2022
Studied period	1 Mar 2011– 31 Jul 2011	1 Mar 2015– 4 Aug 2015	1 Mar 2017– 2 Aug 2017	1 Mar 2019– 3 Aug 2019	1 Mar 2022– 24 Jul 2022
Measured dry matter	Vegetative (leaf+stem), storage organ	Vegetative (leaf+stem), storage organ	Leaf, stem, storage organ	Leaf, stem, storage organ	Leaf, stem, root, storage organ
Grain yield (t ha^{-1})	9.16	8.81	8.63	9.71	11.31
NEE coverage (%)	45.7	46.9	42.6	34.2	47.9
LE coverage (%)	51.0	58.4	61.7	45.7	63.0

²Addendum: site characteristics are different from Chapter 3, these are taken from IRM records while previous ones were estimated with BE-Lon data.

³Addendum: for this study, only the active vegetation period (from 1st March) was considered because biomass is not measured before this date (Table 4.6) and because the coupling between carbon and water fluxes, one focus of this study, is more influential during this period, as shown in the temporal GSA.

During these five seasons, regular measurements of biomass were performed along with continuous measurements of NEE and LE. These flux data were corrected for frequency losses and filtered for low turbulence and nonstationary conditions, contributing to high-quality coverage detailed in Table 4.1. Flux data treatment is described in De Ligne et al. (2010) and Pastorello et al. (2020). Data collection (fluxes, biomass and soil) as well as additional information on the site, measurements, or management activities can be found in Delhez et al. (2025).

2.2. Daisy model

2.2.1. Model description and set-up

Daisy is a crop process-based model simulating carbon, nitrogen and water cycles of the soil–vegetation–atmosphere continuum. Initially published by Hansen et al. (1991), Daisy has since been extensively described (Abrahamsen and Hansen, 2000; Hansen et al., 2012), developed (Plauborg et al., 2010; Holbak et al., 2021), evaluated and compared (Palosuo et al., 2011; Tenreiro et al., 2020; Yin et al., 2020) in the literature. Different modelling options are included in Daisy and must be selected by the modeller depending on the objectives and data availability.

In the present study, the 1D version of Daisy was used with an hourly time resolution. Hourly measurements of air temperature, air vapour pressure, global radiation, wind strength and precipitation were provided as inputs. Water movement in unsaturated soil is described by Richards' equation and, for each soil layer, retention and conductivity curves have been established with the Mualem–van Genuchten model (Mualem, 1976; van Genuchten, 1980). Water drains, located at 70 cm depth in BE-Lon, were explicitly considered (Delhez et al., 2025). Below the soil profile, there is an aquitard layer (i.e., water blocking layer) and an aquifer whose pressure varies according to water table depth measurements also provided as inputs. Potential evapotranspiration is estimated with the FAO56 Penman-Monteith equation, using the reference evapotranspiration ET_0 adjusted to surface cover through bare soil and crop coefficients (Allen et al., 1998; Allen et al., 2006). Water can be evaporated from free water surfaces (canopy interception or ponding), from soil surface or transpired by plants. Actual soil evaporation is governed by the soil hydraulic conductivity, as soil water must be transported to the soil surface, and limited by the potential evaporation. As for the actual transpiration, it is computed together with the entire surface energy balance within the soil-vegetation-atmosphere transfer (SVAT) module (Plauborg et al., 2010). To numerically solve this energy balance, the SVAT module is coupled with the biochemical photosynthesis model of de Pury and Farquhar (1997) and a stomatal conductance empirical model (eq. (4.1)). In this version, the stomatal conductance g_s is based on (Leuning, 1995) and adjusted to account for hydraulic signalling (Plauborg et al., 2010):

$$g_s = g_0 + \frac{g_1 \cdot e^{-\delta|\psi_c|}}{\left(1 + \frac{VPD}{D_0}\right) \cdot (C_s - \Gamma)} A_{net} \quad (4.2)$$

where C_s is the CO₂ concentration at the leaf surface, Γ the CO₂ compensation point, VPD the vapour pressure deficit at the leaf surface, ψ_c the crown water potential (with the related parameter δ) and g_0 , g_1 and D_0 are Leuning parameters.

Compared to Daisy v7.0.7, several modifications related to the diffuse radiation, maintenance respiration and carbon reserve remobilisation were made (Section 6.1) and later integrated into the latest version (v7.1.0).

2.2.2. Model parameters

In our global sensitivity analysis performed on yield, NEE and LE, we demonstrated the significant influence of about 25 parameters out of 200 (Delhez et al., 2025). However, some adjustments to our selection have been made for this present work. The influential parameters related to the phenology, the allocation and the diffuse fraction of solar radiation have already been estimated separately, as direct measurements are carried out at BE-Lon station⁴. Additionally, the temperature scaling constant c_{Vm} and the leaf Rubisco-N fraction were discarded and set to their default value because of their high correlation with other parameters. Conversely, some parameters were added as this study takes new processes into account, such as the photosynthetic contribution of stem and storage organs. Hence, there are 22 parameters included in this study, all described in Table 4.2. Half of these parameters were considered to be cultivar-specific, while the others are site-specific.

⁴Addendum: phenology (i.e., DSRate1, DSRate2, EmrTSum) parameters were fitted based on development stage observations, allocation parameters were estimated by Kim during her master's thesis (Hoang, 2022) and new diffuse parameters are detailed in Section 6.1. The complete parameterisation is available on **GitHub** (Delhez, 2025).

Table 4.2: Model parameters used in this study and their acceptable range. These ranges were established from measurements, literature and the Daisy reference manual. The superscript ^a indicates cultivar-specific parameters that were estimated separately for each growing season.

Parameter	Range	Units	Description	Name in Daisy code
fPSII ^a	0.16-0.5	-	Fraction of PAR effectively absorbed by PSII	alfa
Xn ^a	0.0006-0.002	mol mol ⁻¹ s ⁻¹	Ratio of photosynthetic capacity V _{max} to leaf RubisCO-N	Xn
D ₀ ^a	500-3500	Pa	Leuning empirical coefficient	Do
g ₁ ^a	9-18	-	Leuning stomatal slope	m
g ₀ ^a	0.008-0.02	mol m ⁻² s ⁻¹	Leuning stomatal intercept	b
δ ^a	0-1	-	Empirical constant for hydraulic signalling	delta
SpLAI ^a	0.0144-0.0216	m ² g ⁻¹	Specific leaf area	SpLAI
ShldResC ^a	20-50	%	Capacity of shielded reserves as fraction of stem DM	ShldResC
NII _{crit} ^a	1.26-1.54	-	Stem/leaf partitioning modifier (threshold)	NNI_crit
SOrgPhotEff ^a	0-1	-	Photosynthetic efficiency of storage organ	SOrgPhoEff
StemPhotEff ^a	0-1	-	Photosynthetic efficiency of stem	StemPhotEff
PenPar2	0-5	°C	Root penetration rate parameter (threshold)	PenPar2
σ _{NIR}	0.72-0.95	-	Leaf scattering coefficient of NIR	sigma_NIR
ε _{leaf}	0.94-0.99	-	Leaf emissivity for longwave radiation	epsilon_leaf
k _{net}	0.3-0.5	-	Radiation extinction coefficient	EPext
A _{brunt}	0.5-0.57	-	Brunt parameter (offset)	A
B _{brunt}	0.065-0.075	hPa ^{-1/2}	Brunt parameter (vapour pressure factor)	B
K _c	0.4-0.7	-	Conversion of ET ₀ to bare soil evaporation	EpFactor
K _c	1-1.4	-	Conversion of ET ₀ to crop transpiration	EpFac
K _{sat,1}	0.01-0.05	cm h ⁻¹	Hydraulic conductivity at saturation of first soil layer	K_sat
K _{aquitard}	0.005-0.05	cm h ⁻¹	Hydraulic conductivity at saturation of the aquitard	K_aquitard
Z _{aquitard}	1-2.5	m	Thickness of the aquitard	Z_aquitard

2.3. Multi-objective calibration

2.3.1. Key concepts

Calibrating model parameters while considering multiple objectives simultaneously can be formulated as a minimisation problem (Equation (4.3)):

$$\min \mathbf{F}(\mathbf{x}) = \begin{bmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \\ f_3(\mathbf{x}) \end{bmatrix} \quad (4.3)$$

where $\mathbf{x}$ is a vector of model parameters to be optimised and f_i represents the objective functions. In this study, the objective functions correspond to the relative root mean square error (rRMSE) between modelled and observed values Equation (4.4):

$$f_i(\mathbf{x}) = \frac{\sqrt{\frac{1}{n} \sum_{k=1}^n (y_k - d_k)^2}}{\frac{1}{n} \sum_{k=1}^n d_k} \quad (4.4)$$

Here, y_k and d_k denote the modelled and observed values at time step k for DM ($i = 1$), NEE ($i = 2$) and LE ($i = 3$). Normalising the RMSE by the mean of observed data in Equation (4.4) enables fair comparison across variables of different scales.

As these objectives can be conflicting, the minimisation problem defined in Equation (4.3) typically results in a set of trade-off solutions known as the Pareto-optimal set, rather than a single solution (Deb, 2001). In this configuration, improving one objective cannot occur without degrading at least one of the others. For this reason, these solutions are also referred to as non-dominated solutions. Visualising these non-dominated solutions in the objective space, referred to as the Pareto front, helps to assess the relationship among objectives and identify model structural errors (Efstratiadis and Koutsoyiannis, 2010).

2.3.2. Search algorithm - SMPSO

Particle Swarm Optimisation (PSO) is a population-based optimisation technique inspired by the social behaviour of birds within a flock (Kennedy and Eberhart, 1995). Each potential solution, called a particle i , is characterised by its position and velocity, and a swarm is defined as the population of particles. Aiming to minimise the objective, the particle moves through the search space, balancing between personal exploration (local optimum) and social learning from the swarm (global optimum) (Sharma and Kumar, 2022). The updated position of a particle $\mathbf{x}^{(t+1)}$ is determined by Equation (4.5):

$$\mathbf{x}_i^{(t+1)} = \mathbf{x}_i^{(t)} + \mathbf{v}_i^{(t+1)} \quad (4.5)$$

where $\mathbf{v}_i^{(t+1)}$ is the updated velocity which explicitly expresses the balance between personal and social learning:

$$\mathbf{v}_i^{(t+1)} = w\mathbf{v}_i^{(t)} + c_1r_1 \left(\mathbf{x}_{p_i} - \mathbf{x}_i^{(t)} \right) + c_2r_2 \left(\mathbf{x}_{g_i} - \mathbf{x}_i^{(t)} \right) \quad (4.6)$$

In Equation (4.6), $\mathbf{x}_{p_i}$ is the best position that particle i has visited, $\mathbf{x}_{g_i}$ is the best position that the entire swarm has visited (leader), w is the inertia weight controlling the influence of past velocities, r_1 and r_2 are random numbers drawn from the uniform distribution $U(0, 1)$, and c_1 and c_2 are learning factors determining the relative influence of personal and global experience.

In this study, we employed the SMPSO algorithm, which is specifically designed for multi-objective problems (Nebro et al., 2009). Based on the OMOPSO algorithm (Sierra and Coello Coello, 2005), SMPSO also uses Pareto dominance (Section 2.3.1) and a crowding factor to identify non-dominated solutions. Moreover, it includes a velocity constriction mechanism to prevent the so-called swarm explosion effect, an external archive to store these non-dominated solutions, and the use of polynomial mutation. As suggested by Nebro et al. (2009), the learning factors c_1 and c_2 were drawn from the distribution $U(1.5, 2.5)$ and the mutation probability was set as the inverse of the problem's dimensionality.

2.3.3. Application

The Python-based framework for MOO called jMetalPy (Benítez-Hidalgo et al., 2019) includes SMPSO algorithm and was used in combination with PyDaisy library. For each parameter set (i.e., potential solution) generated by SMPSO, the parameter values were transcribed into Daisy setup files. These include cultivar-specific parameters, with possibly different values for each season, and site-specific parameters that are shared (Table 2). Hence, the model was executed four times, specifically for S15, S17, S19 and S22. The three objective functions (rRMSE) were then computed from these four aggregated runs and passed back to the SMPSO algorithm. Throughout the optimisation process, the hypervolume indicator (referred to as the size of the dominated space) was estimated to evaluate the performance of SMPSO and check for convergence (Guerreiro et al., 2022; Shang et al., 2021). In total, 50000 model simulations were performed with a swarm size of 200 particles.

2.4. Validation

As mentioned in Section 2.1, S11 was not used for this multi-objective calibration but kept for validation. Parameter sets were selected from the Pareto front established with the SMPSO algorithm, and cultivar-specific parameters were taken from S15 as the same cultivar was sown during both seasons. In order to evaluate the performance of Daisy model, four criteria were estimated: (i) the RMSE expressed in the same units as the variable of interest, (ii) the rRMSE for comparison within calibration results,

(iii) the normalised mean error (NME) revealing bias and (iv) the model efficiency (EF) which is a normalised metric. This last criterion is also known as Nash–Sutcliffe Efficiency (NSE) coefficient and is computed as follows:

$$EF = 1 - \frac{\sum_{k=1}^n (y_k - d_k)^2}{\sum_{k=1}^n (d_k - \bar{d}_k)^2} \quad (4.7)$$

In Equation (4.7), y_k and d_k denote the modelled and observed values at time step k , and $\bar{d}_k$ is the mean observed value. The model is perfect when $EF = 1$, while model predictions are as accurate as the mean of observations when $EF = 0$, which is easily interpreted. The validation results are considered acceptable if EF is greater than 0.5 (Dumont et al., 2014).

3. Results

3.1. Pareto front

Non-dominated solutions based on the three objective functions are depicted in Figure 4.1a. The red point indicates the most balanced compromise, defined as the non-dominated solution nearest to the point representing the lowest values across all objectives. The trade-off between DM and NEE is the most clearly defined, as shown in the 2D projection (Figure 4.1b), where the curved Pareto front extends over a large part of the objective space. This 2D front portrays 29% of the solutions from Figure 4.1a, and the other solutions (grey crosses) mainly lie along it. Conversely, the LE–NEE front appears angular and narrower, particularly along the LE axis (Figure 4.1c). Combined with the relatively high rRMSE, it highlights the difficulty in accurately simulating observed LE as well as the limited model responsiveness for this objective.

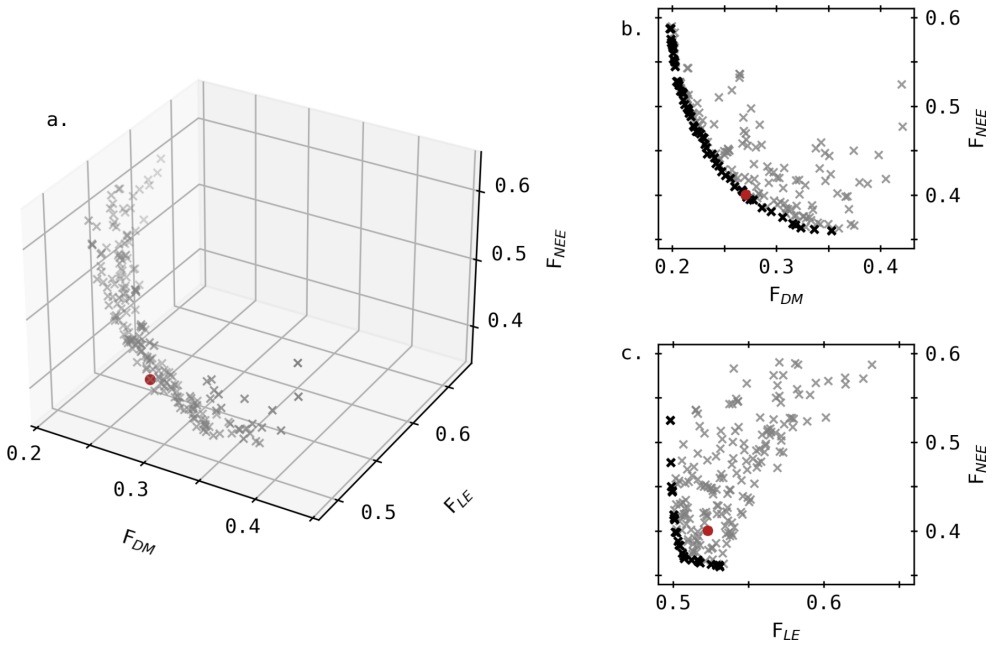


Figure 4.1: Non-dominated solutions in the objective space: (a) 3D Pareto front according to the rRMSE of DM, LE and NEE, and 2D projection of these solutions considering (b) DM and NEE, (c) LE and NEE. Black dots indicate the Pareto front in 2D space, and the red point highlights the most balanced compromise

Values of the most balanced parameter set (i.e., red point) can be found in Section 6.2 (Table 4.4) along with the algorithm convergence indicator (Figure 4.6). In Figure 4.1a, the specific coordinates of this point are (0.27, 0.40, 0.52) which correspond to RMSE values of 0.948 t ha^{-1} , $3.44 \mu\text{mol m}^{-2} \text{ s}^{-1}$ and 62.7 W m^{-2} for DM, NEE and LE respectively, computed across all four growing seasons. In the following sections, the simulated outputs using this parameter set are compared to observed values in terms of dry matter as well as carbon and water fluxes.

3.2. *Dry matter*

In addition to the biomass of individual simulated organs (leaf, stem, storage organs (SOrg) and root), the aboveground vegetative biomass (leaf+stem) was also included in Figure 4.2 as distinct measurements of these two organs were not systematic (Table 4.1). Overall, the simulated dry matter aligns relatively well with observations. Nevertheless, SOrg biomass is consistently underestimated at the end of all growing seasons, resulting in a lower simulated crop yield. Although not shown, predictions of Crop Area Index (CAI) follow a similar pattern, with greater underestimations near the end of the season.

For S15, this underestimation may be attributed to insufficient remobilisation of stem reserves, as indicated by the high simulated stem biomass in July, even greater than the combined leaf and stem observations. However, this explanation does not hold for the other seasons, where stem biomass appears realistic. Beyond the capacity of remobilised reserves, parameters such as the efficiency of this remobilisation (considered fixed in Daisy) as well as contributions from stem and ear to photosynthesis (SOrg-PhotEff and StemPhotEff) may also affect SOrg biomass during the reproductive stage (after anthesis).

3.3. *Fluxes*

As depicted in Figure 4.3, simulated temporal variations follow observed trends, although predictions tend to be more negative (i.e., more CO_2 uptake) during the vegetative stage. This underestimation is particularly evident for S17, also highlighted by the scatter plot, where the regression slope is significantly higher than 1 ($\beta = 1.14$). This bias suggests an overestimation of photosynthesis and/or an underestimation of respiration. Despite this discrepancy, the model accurately simulates the biomass of vegetative organs during this stage. On the other hand, during the reproductive stage (when SOrg is underestimated; Figure 4.2), NEE predictions no longer show a clear bias. This partly explains the observed trade-off between DM and NEE (Figure 4.1b). For instance, increasing the remobilisation of stem reserves during S15 would likely result in a more accurate crop yield, but also in an undesirable increase in NEE as CO_2 is released through this process.

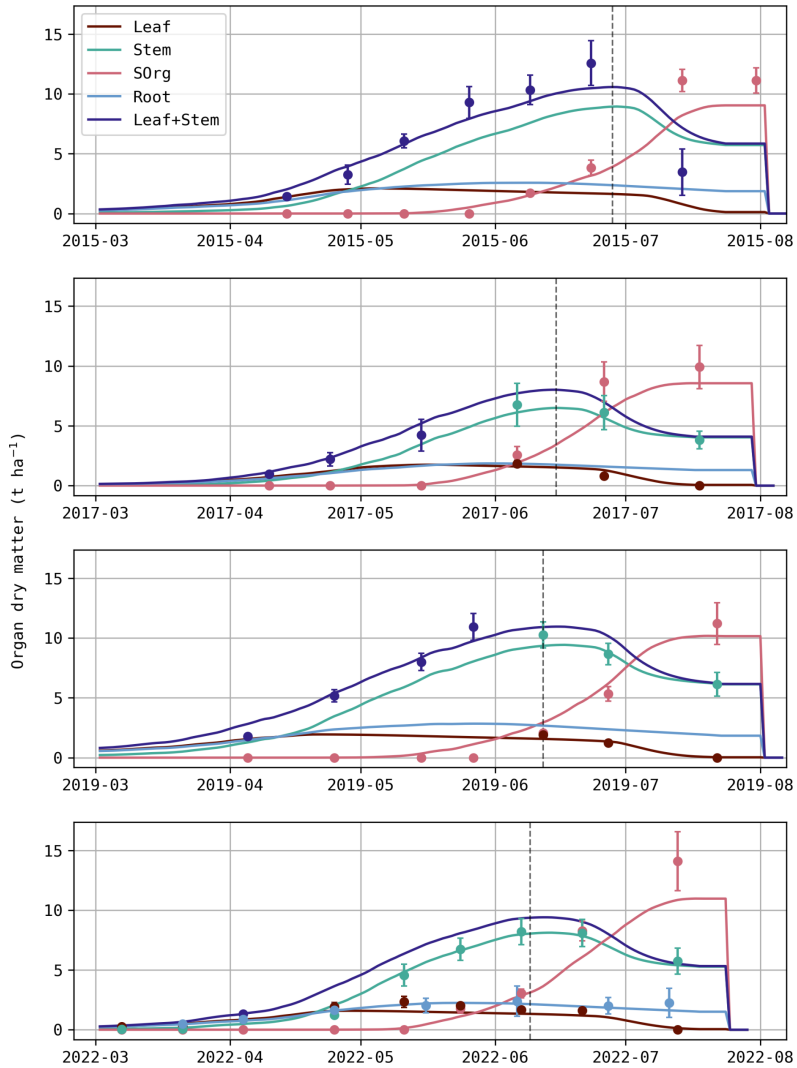


Figure 4.2: Daily evolution of predicted (solid line) and observed (dot) dry matter for each organ (t ha^{-1}). Error bars depicted for the observed dry matter represent the standard deviations and the dashed vertical line indicates the anthesis.

It is also worth noting that Daisy simulates a sudden decrease in NEE at the end of each season, which is not observed. When reaching maturity ($DS = 2$), plant processes are completely stopped, so is the autotrophic respiration. Actually, matured plants continue to respire and contribute to carbon fluxes until harvest⁵.

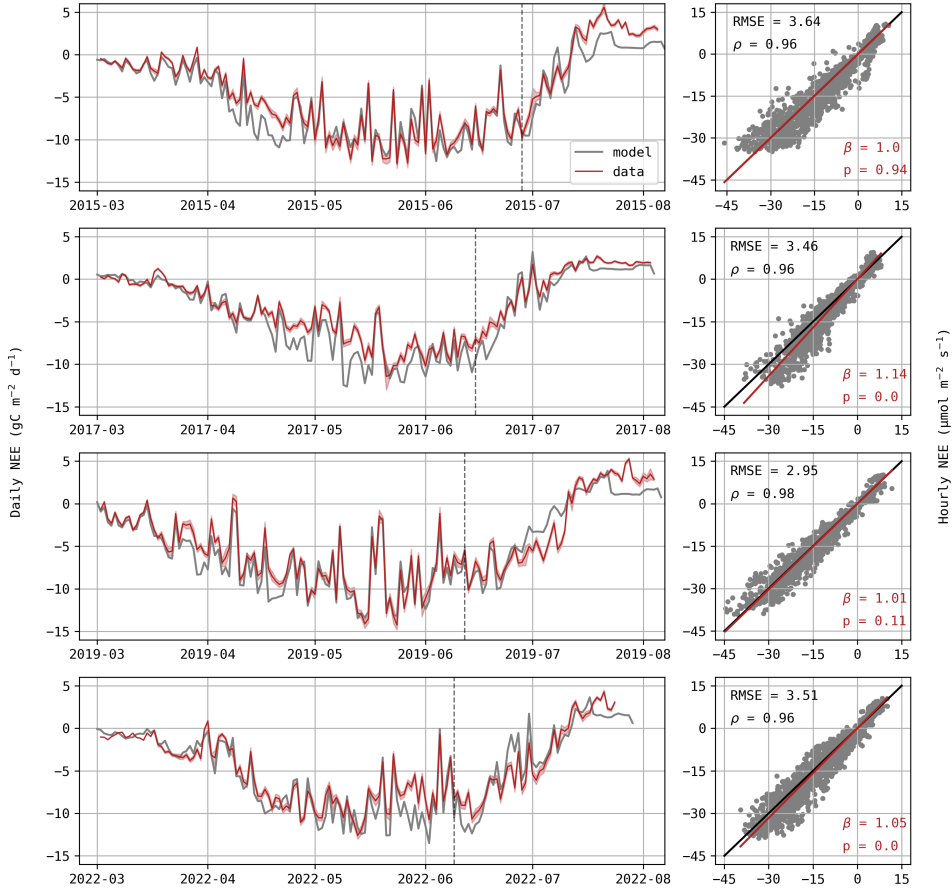


Figure 4.3: Daily NEE ($\text{gC m}^{-2} \text{d}^{-1}$) for each growing season (left) with the red shaded area representing standard deviations of observations. Hourly predictions against observed values of NEE ($\mu\text{mol m}^{-2} \text{s}^{-1}$; right) where observed values are displayed on the x-axis. The p-value indicates if the regression slope β (red) is significantly different from the 1:1 line (black) and ρ is the Pearson correlation coefficient.

As expected from the rRMSE values observed in Figure 4.1, LE fluxes are not well captured by the model. Observed daily fluxes exhibit greater variations, frequently reaching high values or dropping below 50 W m^{-2} while simulated values remain

⁵Addendum: other noteworthy points regarding Figure 4.3. Even if gap-filled data are used for visualisation of daily fluxes, calibration was made with only high-quality data (data coverage in Table 4.1). Standard deviations are the joint uncertainties computed according to Pastorello et al. (2020).

relatively stable (Figure 4.4). This is also illustrated in the scatter plots, where hourly observed data easily reach 600 W m^{-2} , but simulated fluxes never exceed 500 W m^{-2} , resulting in a poor linear agreement between observed and simulated fluxes as indicated by the low value of Pearson correlation coefficients ρ (Figure 4.4). This disagreement is particularly visible in mid-April 2019, with an observed daily average around 150 W m^{-2} in comparison to a prediction of only 100 W m^{-2} . During this period, simulated evapotranspiration equals potential evapotranspiration, suggesting that the plant was not water-limited and that the underestimation stems from deficiencies in energy partitioning rather than water availability.

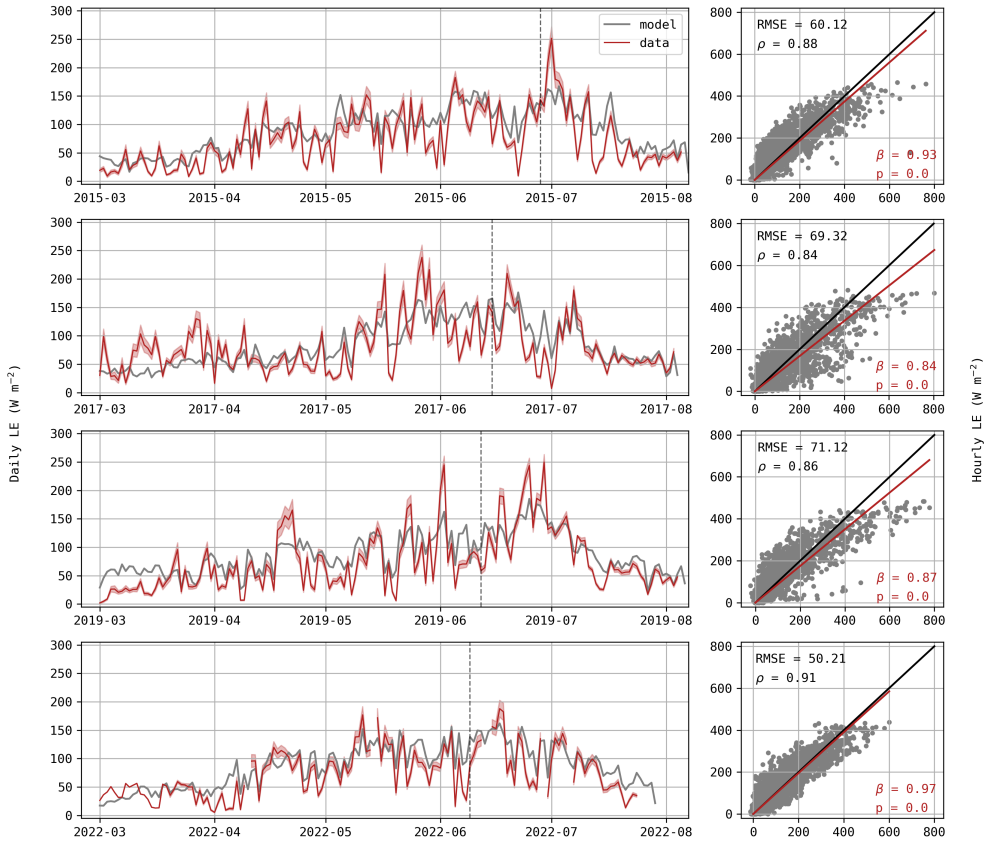


Figure 4.4: Daily LE (W m^{-2}) for each growing season (left) with the red shaded area representing standard deviations of observations. Hourly predictions against observed values of LE (right) where observed values are displayed on the x-axis. The p-value indicates if the regression slope β (red) is significantly different from the 1:1 line (black) and ρ is the Pearson correlation coefficient.

Even though there was no apparent soil water deficit, this period (April 18 – April 22) was still characterised by elevated temperatures and a higher vapour pressure deficit

compared to preceding days. Weather data during this period are depicted in the appendices (Figure 4.7). It does not meet the formal Belgian definition of a heatwave, but the daily mean temperatures were more than 5°C above the 1981–2010 averages. During this 5-day period, the observed stomatal conductance g_s reached extremely high values (Figure 4.5a), associated with an important increase in LE fluxes (Figure 4.5c), while the magnitude of the carbon uptake (GPP) was not affected (Figure 4.5b). These observations reveal a decrease in water use efficiency during this period, indicating that transpiration was intensified with no corresponding increase in carbon assimilation. This trend was not captured by the model, as simulated g_s remained lower than 0.03 m s⁻¹ (Figure 4.5a). The slight increase in predicted g_s during these five days can be explained by the minor increase in carbon uptake (Figure 4.5b).

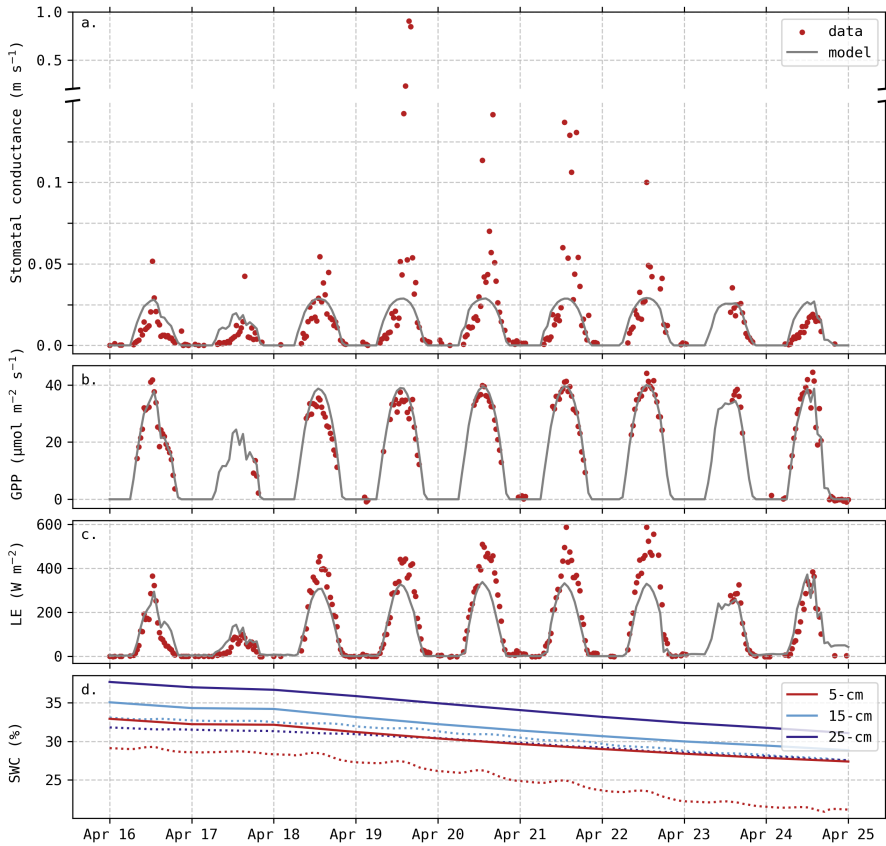


Figure 4.5: Evolution of predicted and observed (a) stomatal conductance g_s , (b) gross primary productivity (GPP), (c) LE fluxes and (d) soil water content (SWC) at three different depths. Solid lines are predictions. Observed g_s was deduced from Penman–Monteith equation, measured fluxes and weather data (Section 6.3). The axis break indicates different scales but does not imply omitted observations.

In addition to the insufficient simulated transpiration, soil evaporation may also be underestimated. During these five days, soil water content at the surface (5 cm depth) decreased by 6.2% whereas the model predicted a decrease of 4.2% (Figure 4.5d). We assume that this difference (2%) is mainly due to an underestimation of soil evaporation rather than drainage as it is limited to the surface layer and because of the particular meteorological conditions. Considering a surface layer from 0 to 10 cm, this is equivalent to a daily contribution of 10.4 W m^{-2} . Hence, the underestimation of soil evaporation can partly explain the difference in LE fluxes observed in Figure 4.4.

3.4. Validation

When using the most-balanced parameter set for S11, NEE is well reproduced by the model with EF greater than 0.8, rRMSE around 40% and NME close to 0 for both time scales (Table 4.3a). Although rRMSE and EF also present acceptable results for DM, it is worth noting that there is an overall underestimation of this variable ($NME = -0.222$).

Table 4.3: Evaluation criteria for S11 using (a) the most-balanced parameter set (red point) and (b) the parameter set minimising F_{LE} . RMSE are expressed in W m^{-2} for LE, in $\mu\text{mol m}^{-2} \text{ s}^{-1}$ for hourly NEE, in $\text{gC m}^{-2} \text{ d}^{-1}$ for daily NEE and in t ha^{-1} for DM. Other criteria have no units.

Variable	Time Resolution	RMSE	rRMSE	NME	EF
(a) Most-balanced parameter set					
LE	Hourly	99.6	0.706	0.203	0.420
	Daily	52.3	0.901	0.551	-0.353
NEE	Hourly	4.21	0.442	-0.00104	0.899
	Daily	1.78	0.383	0.0463	0.870
DM	Daily	2.09	0.387	-0.222	0.807
(b) LE-oriented parameter set					
LE	Hourly	97.3	0.689	0.177	0.447
	Daily	48.6	0.831	0.503	-0.172
NEE	Hourly	4.89	0.514	-0.0925	0.865
	Daily	2.24	0.484	-0.0821	0.795
DM	Daily	2.38	0.441	-0.271	0.749

On the other hand, there is no good agreement between observed and predicted LE, especially when considering a daily time scale, as shown by the four indicators. Even when using the parameter set that minimises F_{LE} (Figure 4.1a), LE remains poorly captured by the model (Table 4.3b). As expected from the Pareto front, this slight improvement in LE predictions is accompanied by a degradation of NEE and DM predictions.

4. Discussion

4.1. Pareto-based calibration

Considering all objectives, the chosen parameter set (red point in Figure 4.1) show satisfactory calibration results, with a total RMSE of 0.948 t ha^{-1} , $3.44 \mu\text{mol m}^{-2} \text{ s}^{-1}$ and 62.7 W m^{-2} for DM, NEE and LE, respectively. Compared with other models, calibrated RMSE values for total biomass are typically between 0.5 and 1.5 t ha^{-1} (Zhang et al., 2020; Dumont et al., 2014; Casanova and Judge, 2008). Regarding NEE, reported RMSE values for daily fluxes range from 1.3 to $1.9 \text{ gC m}^{-2} \text{ d}^{-1}$ (Revill et al., 2019; Senapati et al., 2018; Lehuger et al., 2010). In the present study, the RMSE computed from hourly NEE ($3.44 \mu\text{mol m}^{-2} \text{ s}^{-1}$) corresponds to a RMSE of $1.49 \text{ gC m}^{-2} \text{ d}^{-1}$ when using daily fluxes, which falls in the mentioned range. Casanova and Judge (2008) reported a RMSE of 62.45 W m^{-2} for hourly LE fluxes, and other studies presented values ranging from 24.65 to 48.5 W m^{-2} for daily fluxes (Wang et al., 2024; Liu et al., 2020a; Dutta et al., 2016), while we found 30.74 W m^{-2} using daily averages.

The calibrated parameters are all within the explored range, without relying on extreme values (Table 4.4), indicating a physically plausible solution. It is, however, worth noting that some cultivar-specific parameters have very different values between seasons, such as δ describing the hydraulic signalling for stomatal conductance or the photosynthetic efficiency of non-leaf organs (SOrgPhotEff and StemPhotEff). Such differences may reflect genotypic variability, but they may also be due to environmental factors not represented in the model. This is, for example, the case for the remobilisation reserve ShldResC which can be impacted by genotype and water stress (Ehdaie et al., 2006). The absence or misrepresentation of environmental factors in the model can be compensated by wider variations between cultivars. Depending on the modeller's objective, these parameters might be kept as cultivar-specific while investigating the environmental influences, or constrained across cultivars to improve model parsimony and robustness.

In addition to providing reliable solutions, Pareto-based multi-objective calibration also offers insights into internal model limitations (Kollat et al., 2012). As related by Schoups et al. (2005), the shape of the Pareto front is an indicator of model structural error. Angular fronts (e.g., NEE–LE front) suggest that different objectives can be simultaneously optimised whereas significant trade-offs (curved or linear fronts) may indicate a wrong parameterisation of the model (Wöhling et al., 2013; Efstratiadis and Koutsoyiannis, 2010). The following sections focus on the NEE–DM and

NEE–LE trade-offs and discuss whether the disagreements between observations and model predictions come from uncertainty due to measurement errors or deeper structural issues.

4.2. *Where does the carbon go?*

As shown by the major trade-off in Figure 4.1b, adjusting model parameters to fit NEE fluxes inevitably compromises the simulation of organ DM. The analysis in Sections 3.2 and 3.3 reveals that this would specifically result in an underestimation of biomass. DM during the vegetative stage is well reproduced when simulated NEE is overly negative, and SOrg DM is underestimated when NEE predictions show less bias (Figures 4.2 and 4.3). This was also observed in the validation results, with a consistent underestimation of DM while NEE showed neither over- nor underestimation. Several factors may contribute to this mismatch:

Underestimation of heterotrophic respiration. If so, as respiration is regarded as positive and photosynthesis as negative with the micrometeorological sign convention, NEE predictions would be too negative (as observed). Improving heterotrophic respiration would affect NEE predictions but its influence on DM would be limited, which could weaken the trade-off between these variables. At this study site, Suleau et al. (2011) partitioned soil respiration into its heterotrophic and autotrophic components using soil chambers, from which they derived temperature functions. When comparing their fitted regression to simulated heterotrophic respiration, Daisy appears to underestimate both temperature sensitivity and baseline respiration rate for three growing seasons (Figure 4.8), supporting this first assumption. It should be noted, however, that this regression depends solely on temperature, ignoring the seasonal variation in residue and fertilisation inputs that also affect soil respiration dynamics. Furthermore, heterotrophic respiration is most likely to be underestimated as, during the bare soil period before sowing, NEE (which only consists of soil respiration at that time) is mostly underestimated (Table 4.5). Adjusting soil parameters might reduce this trade-off, but it would require long-term simulations and respiration data from this study site.

Wrong modelling assumptions. Modelling real-world systems comes with simplifications. For instance, in this study, the partitioning schemes of assimilates were derived from S22, since root measurements were only made during that season, as well as early distinction between leaf and stem. These partitioning coefficients were also applied to the other cultivars, but they might be inadequate and partly contribute to this trade-off. If too much assimilated carbon is allocated to the roots at the expense of the stem, the model would underestimate stem DM, which is crucial for grain filling during the reproductive stage. Conversely, as leaves are not directly affected and are the major contributor to photosynthesis, the influence on NEE would be attenuated. Besides this example, many other assumptions could play a role in these results, such as the organ death rates depending only on development stages or the non-dynamic

leaf abscission rate. However, accounting for these within the model would be, in most cases, ineffective as model users usually do not have enough data to support this level of complexity.

Uncertainties and errors in NEE observations. Eddy covariance (EC) data are affected by multiple factors, including instrumental noise, frequency losses and turbulence conditions (Aubinet et al., 2012). To select only high-quality data, they are thoroughly filtered, resulting in low data coverage, as in Table 4.1. Moreover, turbulence conditions are accounted for in the uncertainty estimation rather than affecting the data itself, with an uncertainty related to the friction velocity, an indicator of turbulence strength (Pastorello et al., 2020). However, an additional source of errors has been discussed in relation to the energy balance closure problem (Gao et al., 2019). EC systems show a systematic underestimation of energy fluxes (sensible and latent heat) ranging from 15 to 20%, which is generally attributed to sub-mesoscale organised structures, generated in the daytime convective layer and enhanced by underlying surface heterogeneities (Mauder et al., 2020; Aubinet et al., 2012). While a standard correction method exists for energy fluxes (Pastorello et al., 2020), its application to CO₂ fluxes remains under active research (Mauder et al., 2024). Some studies suggest that CO₂ fluxes may also be underestimated (Gao et al., 2019; Mauder et al., 2010), though Liu et al. (2024a) found that the bias rather depends on soil water conditions. At BE-Lon, this potential underestimation of NEE is supported by the crop carbon budget previously estimated (Buysse et al., 2017). When combining NEE and field measurements (harvest, residues and inputs), they found that the study site continuously loses an unexpectedly large amount of carbon, depleting the soil much faster than recently observed (Dumont et al., 2025). This highlights that, beyond random error estimates, systematic biases in NEE measurements may propagate into model calibration and interpretation. As Beven (2019) emphasises, observational datasets should not be treated as absolute truth, and acknowledging these uncertainties is important when designing calibration frameworks or interpreting model evaluations.

4.3. Structural limitations in simulating LE

When there is no evaporation from free water surfaces, the surface water balance in Daisy can be summarised as:

1. Computation of potential evapotranspiration (PET) using the FAO56 equation.
2. Partitioning of PET between potential soil evaporation and plant transpiration according to canopy cover.
3. Computation of actual soil evaporation, depending on potential soil evaporation and soil water availability.
4. Numerical resolution of Farquhar–Leuning models simultaneously with the SVAT module (surface energy balance) to obtain actual transpiration, surface temperatures and carbon assimilation.

Model limitations may arise from this workflow in two ways. First, the evapotranspiration (ET) is constrained by FAO56 PET which assumes a fixed stomatal conductance (Allen et al., 2006). Although it is widely used in crop modelling, this simplification can reduce the accuracy of ET estimations (Liu et al., 2023b; Ghiat et al., 2021). By considering a constant g_s for PET, simulated ET can be severely limited when stomata are actually wide open. Conversely, when stomata are closed, PET is overestimated and can therefore lead to higher soil evaporation than observed. This may partly explain the lack of temporal variation observed in Figure 4.4 and the high values of rRMSE (Figure 4.1c).

Second, soil evaporation (E_{soil}) is computed outside the iteration loop that couples the SVAT module with the Farquhar–Leuning models. It is constrained either by soil water availability or by the potential evaporative demand, depending on which is limiting. By contrast, fully coupled models such as the CLM model calculate resistance-based E_{soil} simultaneously with transpiration and sensible heat fluxes (Swenson and Lawrence, 2014). This ensures that E_{soil} is driven by microclimate conditions (e.g., canopy air vapour pressure) and reinforces the mechanistic coupling between the surface energy and water balances. However, the appropriate formulation of resistance-based E_{soil} remains an active research area, as recent studies continue to refine its parameterisation and physical basis (Schulz and Vogel, 2020; Lehmann et al., 2018).

Beside these workflow aspects, the relatively narrow Pareto shape (Figure 4.1c) suggests the presence of equifinality, i.e., multiple parameter sets produce equally good results (Her and Seong, 2018). This likely reflects compensatory interactions between soil evaporation and plant transpiration. Since PET is partitioned by canopy cover, parameter changes that alter canopy development can redistribute PET between the two components while leaving total PET unaffected. Under non-stressed water conditions, the ecosystem would meet this evaporative demand, and total ET (i.e., LE outputs) would remain unchanged as well. This masking effect underscores the well-known challenge of ET partitioning in ecosystem modelling, further complicated as eddy covariance systems do not distinguish between soil evaporation and transpiration (Berg and Sheffield, 2019; Stoy et al., 2019; Scott and Biederman, 2017). Recent methods, such as flux mapping, have been developed to better understand model internal fluxes leading to equifinality (Khatami et al., 2019).

As depicted by Figure 4.5, discrepancies in LE predictions were especially evident under elevated temperatures and high VPD. While these may partly stem from limitations mentioned above, they also point to deeper issues in the coupling between Farquhar and Leuning models and particularly in how it responds to atmospheric drivers.

4.4. Coupling of carbon and water exchanges

Stomatal behaviour plays a central role in plant regulation of water loss and carbon uptake, and has therefore been extensively studied (Damour et al., 2010). While it is

well established that mild edaphic drought induces a decrease in carbon assimilation by reducing the stomatal aperture (Beauclaire et al., 2024b), plant responses to heat-waves and high atmospheric demand are less evident. Most studies report reduced g_s under high VPD (Grossiord et al., 2020; Bourbia and Brodribb, 2024), aligning with the theoretical predictions of stomatal models (Sabot et al., 2022). On the other hand, high temperatures seem to trigger stomatal opening to promote transpiration cooling (Urban et al., 2017a), but reported results vary greatly among species (Wang et al., 2026; Moore et al., 2021). Under the combined effect of high temperature and VPD, Marchin et al. (2022) observed a significant increase in g_s for two well-watered species, interpreting this as a strategy to prevent leaf overheating via enhanced LE loss without any increase in carbon assimilation. They later confirmed that this behaviour, referred to as stomatal decoupling, is not restricted to well-watered species (Marchin et al., 2023).

This stomatal decoupling aligns with ecophysiological studies, highlighting the role of non-stomatal factors during photosynthesis. Inside the leaf, CO_2 diffuses through airspaces and membranes to reach the sites of carboxylation inside chloroplasts, whereas H_2O moves from the xylem network to the stomata (Flexas et al., 2012; Sack and Holbrook, 2006). These different pathways can be affected independently, where carbon assimilation can be restricted by non-stomatal factors, often dominated by mesophyll conductance (Flexas et al., 2012). Over the last decade, these non-stomatal limitations have received increased attention, especially under water-stressed conditions (Nadal and Flexas, 2018; Gago et al., 2020). Based on leaf gas exchange measurements, experimental studies proved that these limitations should be considered in leaf models linking photosynthesis and transpiration (Yang et al., 2019; Beauclaire et al., 2024b; Chen et al., 2025). Despite that, these complex processes are still not fully understood, and hence barely integrated into crop or terrestrial models (Vidale et al., 2021). As an example, an empirical equation for the mesophyll conductance was implemented in the land surface model JSBACH (Knauer et al., 2019). The authors extensively discussed the environmental drivers, the modelling implications, as well as the effects on the predicted fluxes in a subsequent paper (Knauer et al., 2020).

These non-stomatal limitations, or stomatal decoupling, are not modelled in Daisy. Based on stomatal coupling (Equation (4.2)), the increase in VPD reduced the predicted slope between carbon assimilation and g_s . Consequently, the model tended to underestimate g_s and LE fluxes and overestimated sensible heat, leading to a misrepresentation of energy partitioning under such conditions. On the other hand, observations show that plants likely opened their stomata, promoting water loss, while carbon assimilation did not increase accordingly. This stomatal decoupling was particularly visible in April 2019, as the heatwave lasted several days, but also appeared during shorter warm periods, suggesting a recurrent plant strategy. Future work should (i) continue the effort in better understanding the mechanisms of non-stomatal limitations affecting carbon assimilation and (ii) incorporate these mechanisms in process-based

models, particularly under such conditions.

5. Conclusion

In this study, we employed a Pareto-based multi-objective calibration approach to optimise the Daisy soil–plant–atmosphere model, focusing on three key objectives (DM, NEE and LE). The SMPSO algorithm successfully identified parameter sets that balanced these objectives within realistic bounds. Furthermore, this methodology also offered valuable insights into model behaviour and inherent limitations, as particular trade-offs between the objectives were revealed. Notably, the strong compromise between DM and NEE suggests possible wrong parameterisations of the model and/or biases in observational EC data. Moreover, the LE–NEE trade-off indicates issues of equifinality which underlines the challenging partitioning of evapotranspiration. The inaccuracy of LE predictions was also discussed, underscoring the oversimplification of FAO56 Penman-Monteith method.

Additionally, the model struggled to reproduce observed increases in transpiration during heatwave conditions, highlighting deficiencies in simulating stomatal responses and in the coupling between carbon and water fluxes. These limitations are particularly relevant given the increasing frequency and intensity of heatwaves under climate change, which can significantly impact ecosystem dynamics. The influence of heatwaves and underlying mechanisms of stomatal decoupling need to be further investigated to improve the simulation of carbon and energy fluxes.

Overall, this work illustrates how multi-objective calibration can go beyond parameter estimation to critically assess model assumptions and guide future improvements. Addressing the structural limitations identified here – particularly in ET partitioning and (non-)stomatal regulation – could strengthen the ability of Daisy and similar crop models to capture ecosystem responses under changing climate conditions.

6. Appendices

6.1. Appendix A: Daisy modifications

Diffuse fraction. The diffuse fraction of global radiation f_d was estimated using the optical air mass and assuming a cloudless sky (Appendix 1 of de Pury and Farquhar (1997)). A second modelling option for estimating f_d , adapted for cloudy skies, was implemented. Based on Ridley et al. (2010), f_d depends on the hourly and daily clearness index (resp. k_t and K_t), the apparent solar time (AST) and the solar angle α :

$$f_d = \frac{1}{1 + e^{\beta_0 + \beta_1 k_t + \beta_2 AST + \beta_3 \alpha + \beta_4 K_t}} \quad (4.8)$$

As both diffuse and global radiation are measured at BE-Lon, the five β parameters have been estimated with the Nelder–Mead method, considering the RMSE metric as an objective function. This method has been applied to 10 years of measurements (2014–2023), covering the entire duration of the case study. The resulting parameters ($\beta_0, \beta_1, \beta_2, \beta_3, \beta_4$) are respectively equal to -4.8094, 5.4735, 0.020702, 0.099970 and 1.3944 (RMSE for $f_d = 0.164$).

Maintenance respiration. Respiration required to maintain existing biomass is defined as maintenance respiration. In Daisy, the maintenance respiration of an organ R_m^{org} is proportional to its dry weight W^{org} :

$$R_m^{\text{org}} = r_m^{\text{org}} \cdot f(T) \cdot W^{\text{org}} \quad (4.9)$$

where r_m^{org} is the maintenance respiration coefficient of the organ and $f(T)$ is a temperature function. In addition to temperature dependence, it was demonstrated that mature or senescing tissues required lower maintenance respiration than younger tissues (Boote et al., 2013). Maintenance respiration declines near the end of the growing season due to a significant fraction of dead cells and metabolically inactive long-term storage (Amthor, 2025). To account for this, a second dependency $f(DS)$ was added into Equation (4.9) and is a user-defined function of development stage. This more realistic dependence was added to verify whether its consideration impacted the trade-off between DM and NEE, which was not the case.

Remobilisation. After anthesis, carbon reserves stored in the stem can be mobilised to support grain filling. The remobilisation equations in Daisy were modified to account for both remobilisation efficiency and the temporal dynamics of the remobilisation rate. This rate peaks around 20 days after anthesis before declining, resulting in a sigmoid-shaped depletion of stem reserves (Liu et al., 2020c; Ehdaie et al., 2008). Similarly, this process was also modified to better match observations and verify whether it impacted the trade-off between DM and NEE, which was not the case.

6.2. Appendix B: SMPSO results

Figure 4.6: Hypervolume indicator with increasing iterations. The red line corresponds to the solutions presented in this study and the grey line is a previous attempt with less iterations (200 iterations, hence 40 000 simulations).

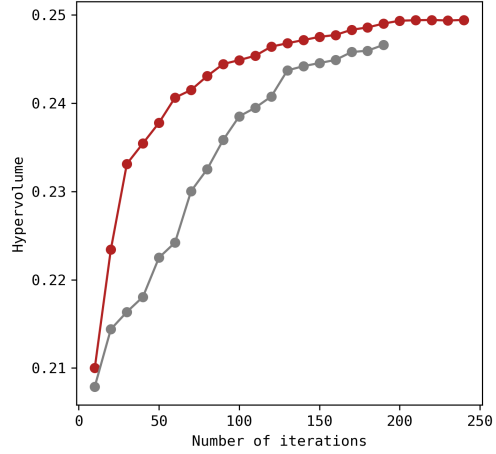


Table 4.4: Most balanced parameter set among non-dominated solutions (red point).

Parameter	S15	S17	S19	S22	Units
fPSII	0.3668	0.3291	0.3645	0.4009	-
Xn	7.929×10^{-4}	7.550×10^{-4}	1.076×10^{-3}	6.835×10^{-4}	$\text{mol mol}^{-1} \text{s}^{-1}$
D ₀	3354	2820	1596	2820	Pa
g ₁	10.54	14.87	14.79	16.79	-
g ₀	0.01335	9.079×10^{-3}	0.01658	0.01324	$\text{mol m}^{-2} \text{s}^{-1}$
δ	0.3635	0.1940	0.4816	0.8232	-
SpLAI	0.01598	0.02103	0.02143	0.01522	$\text{m}^2 \text{g}^{-1}$
ShldResC	49.45	47.60	41.98	42.54	%
NII _{crit}	1.373	1.470	1.444	1.346	-
SOrgPhotEff	0.7227	0.2565	0.1808	0.6703	-
StemPhotEff	0.09723	0.7164	0.2039	0.7606	-
PenPar2		4.822			°C
σ _{NIR}		0.8926			-
ε _{leaf}		0.9825			-
k _{net}		0.3572			-
A _{brunt}		0.5548			-
B _{brunt}		0.06806			$\text{hPa}^{-1/2}$
K _c		0.4724			-
K _c		1.106			-
K _{sat, l}		0.04520			cm h^{-1}
K _{aquitard}		0.03667			cm h^{-1}
Z _{aquitard}		1.974			m

6.3. Appendix C: Determination of stomatal conductance

According to the Penman–Monteith equation, the latent heat flux (LE) can be expressed as follows:

$$LE = \frac{\Delta (R_n - G) + \frac{\rho_a c_p VPD}{r_a}}{\Delta + \gamma \left(1 + \frac{r_s}{r_a}\right)} \quad (4.10)$$

where R_n is the net irradiance (W m^{-2}), G is the ground heat flux (W m^{-2}), VPD is the vapour pressure deficit (Pa), ρ_a is the dry air density (equal to 1.22 kg m^{-3}), c_p is the specific heat capacity of air (equal to $1013 \text{ J kg}^{-1} \text{ }^\circ\text{C}^{-1}$) and r_s is the stomatal resistance ($r_s = g_s^{-1}$). The slope of the saturation vapour pressure with temperature Δ can be estimated based on vapour pressure at saturation $e^*(T_{\text{air}})$:

$$\Delta = \frac{4098 e^*(T_{\text{air}})}{(T_{\text{air}} + 237.3)^2} \quad (4.11)$$

The psychrometric constant γ is a function of atmospheric pressure P :

$$\gamma = \frac{c_p P}{0.622 \cdot 2.45 \cdot 10^6} \quad (4.12)$$

And finally, the atmospheric resistance r_a is composed of the aerodynamic and boundary layer resistances:

$$r_a = \left(\frac{u}{u_*}\right)^2 + 6.2 u_*^{-0.67} \quad (4.13)$$

As LE, G , R_n , VPD, the air temperature T_{air} , P , the wind velocity u , the friction velocity u_* are directly measured or at least computed within the ONEFlux pipeline (Pastorello et al., 2020), the stomatal resistance can be determined by combining Equations (4.10) to (4.13).

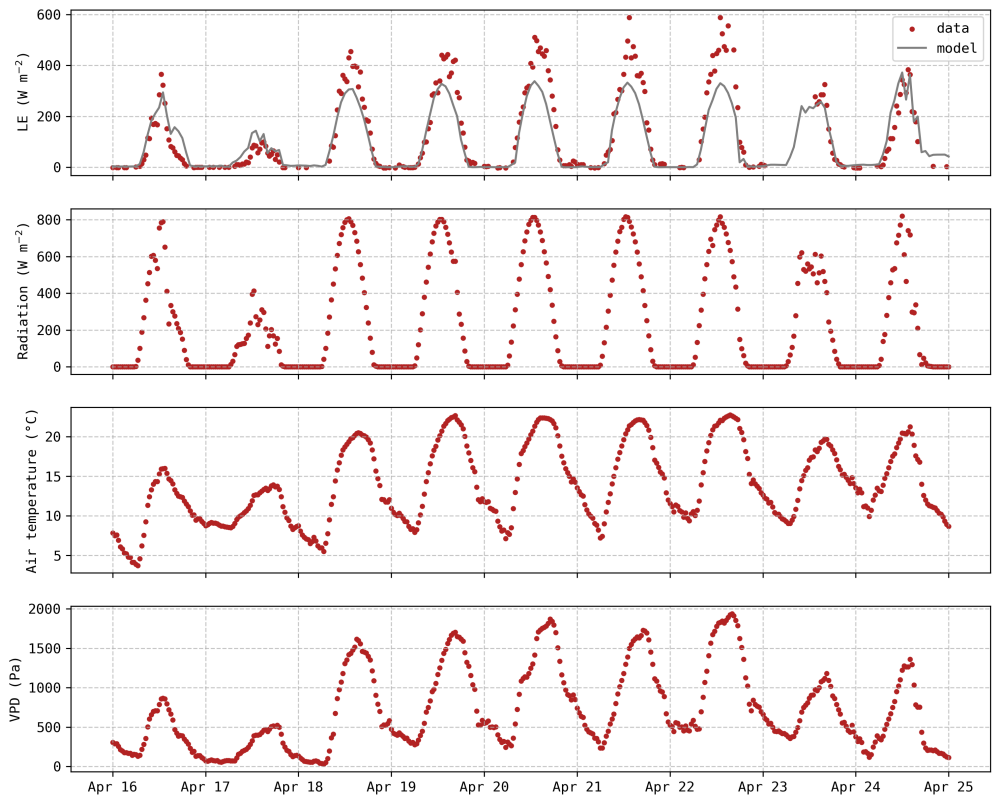


Figure 4.7: Hourly evolution of latent heat flux predictions (grey) and observations (red) along with meteorological data (incoming shortwave radiation, air temperature and VPD).

6.4. Appendix D: Heterotrophic respiration

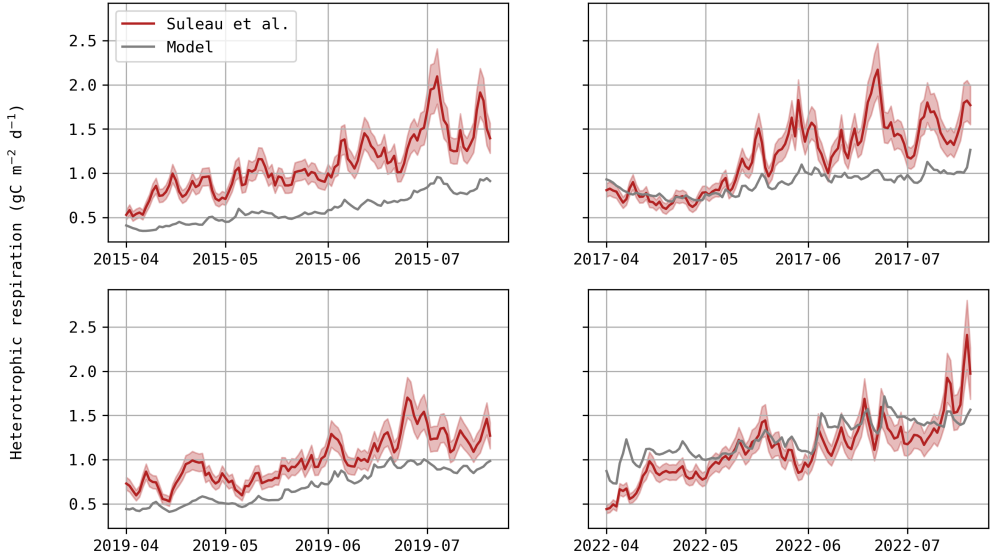


Figure 4.8: Daily evolution of heterotrophic respiration ($\text{gC m}^{-2} \text{d}^{-1}$) – model predictions (grey) and estimations based on the temperature function fitted by Suleau et al. (2011; red).

Table 4.5: Evaluation criteria regarding daily NEE during the bare soil period before sowing. RMSE and ME are expressed in $\text{gC m}^{-2} \text{d}^{-1}$ and other criteria have no units. S11 was simulated with the most-balanced parameter set, and cultivar-specific parameters were taken from S15.

Season	RMSE	rRMSE	ME	NME
S11	0.484	0.376	-0.237	-0.184
S15	0.320	0.308	0.0144	0.0139
S17	0.736	0.422	-0.0493	-0.0282
S19	0.228	0.190	-0.0484	-0.0403
S22	0.622	0.289	-0.490	-0.228

7. Addendum

Table 4.6: Measurements (mean and standard deviation) of dry matter at BE-Lon (tDM ha⁻¹).

Date	Leaf-Stem	Leaf	Stem	Ear	Dead leaves	Root
27-04-2011	4.36 ± 0.197					
15-05-2011	10.6 ± 1.05					
20-06-2011	12.4 ± 0.866			5.04 ± 0.070		
14-04-2015	1.44 ± 0.085					
28-04-2015	3.24 ± 0.80					
11-05-2015	6.07 ± 0.57					
26-05-2015	9.29 ± 1.32					
09-06-2015	10.3 ± 1.23			1.70 ± 0.165		
23-06-2015	12.6 ± 1.87			3.82 ± 0.632		
14-07-2015	3.47 ± 1.94			11.1 ± 0.918		
31-07-2015				11.1 ± 1.06		
10-04-2017	0.966 ± 0.232				0.134 ± 0.050	
24-04-2017	2.20 ± 0.556				0.204 ± 0.045	
15-05-2017	4.22 ± 1.33				0.316 ± 0.125	
06-06-2017		1.84 ± 0.286	6.76 ± 1.80	2.58 ± 0.679	0.969 ± 0.487	
26-06-2017		0.803 ± 0.138	6.11 ± 1.43	8.69 ± 1.65	1.47 ± 0.351	
18-07-2017			3.81 ± 0.743	9.92 ± 1.80	1.34 ± 0.222	
05-04-2019	1.79 ± 0.196				0.715 ± 0.424	
25-04-2019	5.17 ± 0.520				1.15 ± 0.308	
15-05-2019	8.00 ± 0.722				1.19 ± 0.536	
27-05-2019	10.9 ± 1.11				1.90 ± 0.267	
12-06-2019		1.92 ± 0.261	10.3 ± 1.09	2.06 ± 0.232	3.25 ± 0.484	
27-06-2019		1.23 ± 0.228	8.66 ± 0.889	5.35 ± 0.606	1.80 ± 0.401	
22-07-2019			6.14 ± 1.00	11.2 ± 1.75	2.97 ± 0.654	
07-03-2022		0.251 ± 0.063	0.035 ± 0.006			
21-03-2022		0.330 ± 0.06	0.067 ± 0.026		0.055 ± 0.014	0.488 ± 0.187
04-04-2022	1.31 ± 0.181				0.101 ± 0.021	0.858 ± 0.227
25-04-2022		1.91 ± 0.354	1.21 ± 0.145		0.117 ± 0.012	1.64 ± 0.568
11-05-2022		2.33 ± 0.46	4.57 ± 0.905		0.538 ± 0.116	
16-05-2022						2.02 ± 0.616
24-05-2022		2.03 ± 0.115	6.71 ± 0.928	1.75 ± 0.371	1.02 ± 0.178	
07-06-2022		1.67 ± 0.194	8.19 ± 1.09	3.04 ± 0.364	0.99 ± 0.109	2.39 ± 1.27
21-06-2022		1.60 ± 0.231	8.09 ± 1.13	8.26 ± 0.819	1.35 ± 0.068	
27-06-2022						2.00 ± 0.696
13-07-2022			5.74 ± 1.08	14.1 ± 2.45	1.99 ± 0.51	2.25 ± 1.20

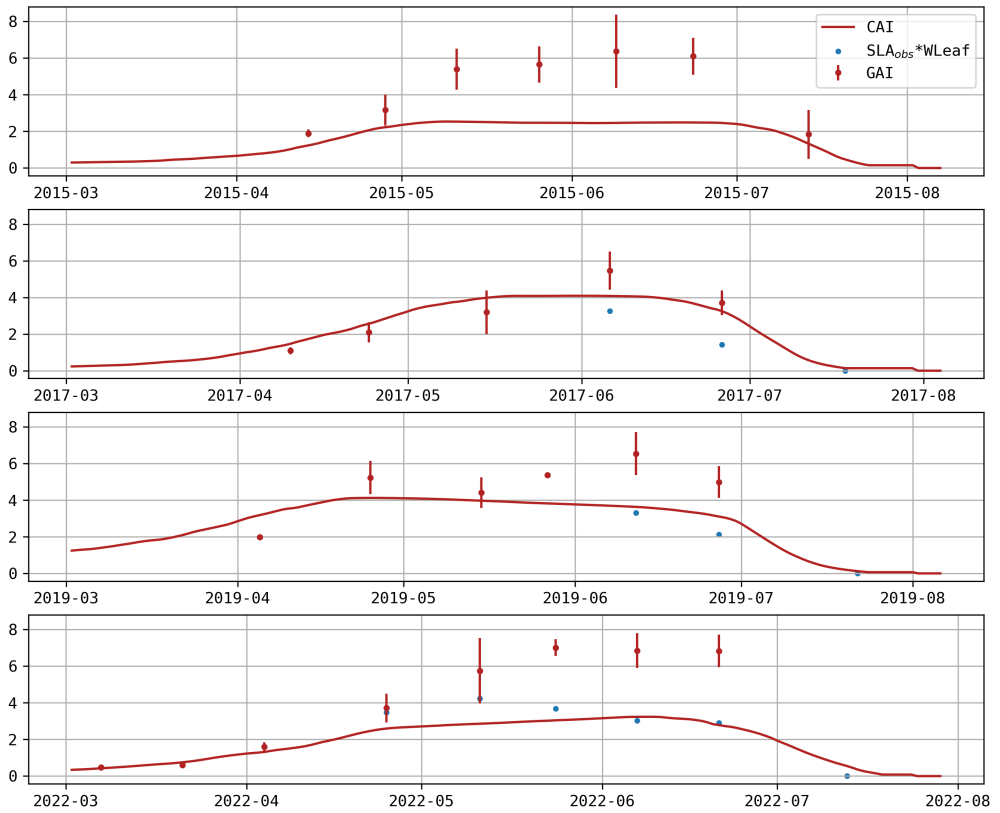


Figure 4.9: Predicted crop area index (CAI) and observed green area index (GAI; $\text{m}^2 \text{m}^{-2}$).

**Using SIF data as model input to
mechanistically model photosynthesis:
Is it worth it?**

Preamble. The photosynthesis representation in Daisy, as described in Chapter 2 and applied throughout Chapters 3 and 4, is based on the FvCB biochemical model. While widely used, this formulation relies on multiple assumptions and thus has several limitations. An alternative approach has recently emerged, namely the mechanistic light response (MLR) model proposed by Gu et al. (2019). Based on measurements of sun-induced chlorophyll fluorescence (SIF), this model estimates the actual electron transport rate, thereby bypassing the high parameterisation of the FvCB model. Another key advantage is that the ecophysiological responses to environmental stress are already embedded in the SIF signal itself rather than being explicitly represented within the model structure. Chapter 5 takes advantage of SIF measurements conducted at BE-Lon in 2022 to integrate the MLR approach into Daisy and compare it against the FvCB model, using the same multi-objective calibration methodology as in Chapter 4. Following on from the previous chapter, this present chapter aims to answer two questions: Does replacing the FvCB model with the MLR approach improve the simulation of NEE and LE for winter wheat? Does the trade-off between dry matter, NEE and LE change depending on the photosynthesis approach?

For this fifth chapter, I made amendments to Daisy code to enable new model inputs (i.e., SIF) and integrate the MLR model, implemented the calibration method, analysed the results and wrote the manuscript. Quentin Beauclaire provided the dataset, contributed to the conceptualisation as well as the interpretation of the results. Bernard Longdoz supervised the research, also helped with the interpretation of the results and reviewed the manuscript.

Delhez, L., Beauclaire, Q., and Longdoz, B.: Using SIF data as model input to mechanistically model photosynthesis: Is it worth it? *In prep.*

1. Introduction

Accurate quantification of gross primary productivity (GPP) is central to our understanding of terrestrial carbon cycling and the responses of ecosystems to environmental stress. At the canopy scale, photosynthesis is commonly simulated using the biochemical model of Farquhar, von Caemmerer and Berry (FvCB), which describes CO₂ assimilation as co-limited by Rubisco activity and RuBP regeneration through electron transport (Farquhar et al., 1980). Although mechanistically grounded, this framework relies on multiple assumptions. To name just a few, there are the Arrhenius temperature dependences of some model parameters, the steady-state regime of photosynthesis, a uniform irradiance in terms of wavelength, electron transport being entirely linear and the empirical relationship between the actual electron transport J and PAR (Wang et al., 2020; Jans et al., 2025; Yin and Struik, 2009). Moreover, the FvCB model represents ecophysiological responses to stress (e.g., stomatal closure under drought, heat damage to photosystem II, photoprotection) through explicit parameterisations that must be calibrated independently. These constraints limit the portability of the approach and may introduce propagated uncertainties when applied under variable environmental conditions.

An alternative source of information on the photosynthetic activity of vegetation comes from the chlorophyll fluorescence emission. Although both photosystems emit fluorescence, they differ in their spectral properties, functional roles and contribution to the total fluorescence emission spectrum. Photosystem II (PSII), excited predominantly by wavelengths below 680 nm, is responsible for the oxidation of water and the release of molecular oxygen, thereby initiating the linear electron transport chain. Photosystem I (PSI), preferentially excited by red and far-red wavelengths above 680 nm, uses the downstream electrons to reduce NADP⁺ to NADPH (Jans et al., 2025). Their fluorescence emission spectra partly overlap, but PSII dominates in the red peak (685 nm) and remains the primary contributor in the far-red (740–760 nm). Whereas PSI fluorescence carries little information on photosynthetic regulation (being largely temperature-dependent and insensitive to other pathways of energy dissipation), the PSII emission is an essential informative component for photosynthesis (Porcar-Castell et al., 2021).

When chlorophyll *a* molecules associated with PSII absorb photons, the excited electrons must eventually relax to their ground state (i.e., a process called deactivation). It can be done through three competing energy pathways: photochemical quenching (PQ) promoting the electron transport and CO₂ fixation, thermal dissipation defined as non-photochemical quenching (NPQ), and re-emission as fluorescence (F) (Porcar-

Castell et al., 2021; Mohammed et al., 2019). The fluorescence quantum yield Φ_F is accordingly defined as the ratio of the fluorescence emission rate to the sum of all deactivation rates. Similarly, the photochemical quantum yield of PSII Φ_{PSII} reflects the fraction of absorbed energy directed into photochemistry and Φ_{NPQ} is the fraction redirected into heat dissipation as a photoprotective mechanism (Murchie and Ruban, 2020). Because PQ, NPQ and F are complementary pathways, any change in photosynthetic activity is reflected in the fluorescence emission of PSII, making it a sensitive and integrative indicator of canopy photosynthetic activity.

Chlorophyll fluorescence can be measured at the leaf level using active techniques, where dedicated fluorometers with artificial excitation sources can estimate the maximum photochemical quantum yield $\Phi_{\text{PSII,max}}$ under controlled environmental conditions (Kalaji et al., 2014). Note that, contrary to Φ_{PSII} which is the effective quantum yield of PSII, $\Phi_{\text{PSII,max}}$ represents the quantum yield when all reaction centres of PSII are open, thus under dark conditions. At the canopy scale, the passive measurement of sun-induced chlorophyll fluorescence (SIF) is more practical. SIF is the fluorescence emitted by vegetation under natural solar illumination, without any artificial excitation. Following a multi-step correction procedure accounting for PSI/PSII partitioning, canopy escape probability and spectral broadband integration, it is possible to estimate the fluorescence emitted by PSII from SIF measurements above the canopy.

The mechanistic link between SIF and GPP provides a compelling justification for using SIF as a model input rather than merely a diagnostic variable. SIF already encodes the effects of environmental stressors on photosynthetic efficiency: stomatal closure, NPQ induction and photoinhibition are all included in the fluorescence signal. This property circumvents the need to parameterise individual stress functions within a model and has led to the development of direct SIF-based GPP estimators at both the leaf and canopy scales (Liu et al., 2022b). One such approach is the mechanistic light response (MLR) model proposed by Gu et al. (2019), linking SIF emitted by PSII and GPP through the actual electron transport rate. This model requires fewer parameters, does not rely on temperature response functions for $V_{c,\text{max}}$ and J_{max} , and does not need to explicitly account for ecophysiological responses to environmental stress as they are already embedded in the SIF signal.

In this chapter, we integrate the MLR model into the Daisy soil-plant-atmosphere model (Hansen et al., 2012; Plauborg et al., 2010) and evaluate its performance against the FvCB formulation for a winter wheat crop at BE-Lon station. This chapter addresses three related questions: (i) does replacing the FvCB model with the MLR approach improve the simulation of net ecosystem exchange (NEE) and latent heat flux (LE) for winter wheat? (ii) does the trade-off between dry matter, NEE and LE observed in Chapter 4 change depending on the photosynthesis formulation? and (iii) can the MLR model be considered a robust alternative to FvCB-based approaches when integrated in a complete modelling framework?

2. Materials and methods

2.1. Study site and measurements

The BE-Lon station, where previous studies were conducted (Chapters 3 and 4), is an ICOS monitoring site equipped with an eddy covariance system and a micrometeorological station since 2004. In 2022, when winter wheat (*Triticum aestivum* L. Skyscraper) was growing, a FloX instrument (JB Hyperspectral, Düsseldorf, Germany) was installed above the canopy. Comprising two spectrometers, this device measures the solar irradiance with upward optical fibers and the upwelling radiance with downward fibers, covering the range between 650 and 800 nm (Beauclaire et al., 2024a). This upwelling radiance contains both reflected canopy radiance and fluorescence emissions (Cendrero-Mateo et al., 2019). In order to decouple the reflectance and SIF, the spectral fitting method (SFM) was used considering the O₂-A absorption band (Beauclaire et al., 2024a). In this band (760 nm), the SIF signal is stronger and less affected by chlorophyll reabsorption within the canopy (Chang et al., 2024; Chang et al., 2020). This signal is referred to as SIF_{TOC} hereafter, since it corresponds to the fluorescence (at 760 nm) at the top of the canopy.

Three distinctions must be made between SIF_{TOC} and the SIF emitted by the PSII inside the leaves (SIF_{TOT}) which is required for the MLR model. Firstly, the fluorescence measured by the FloX originates from both photosystems, so the contribution of each photosystem within SIF_{TOC} needs to be assessed. Secondly, as for light that can be scattered and reflected before reaching the leaves, the fluorescence can also be scattered and reabsorbed before reaching the top of the canopy. Lastly, SIF_{TOC} was determined in a specific absorption band (760 nm), hence it needs to be integrated over the broadband chlorophyll fluorescence spectrum. To account for these distinctions, three conversion factors were estimated as follows (Beauclaire et al., 2024a; Liu et al., 2022b):

$$SIF_{TOT} = \frac{SIF_{TOC} \cdot f_{SIF,PSII} \cdot f_{\lambda}}{f_{esc}} \quad (5.1)$$

where $f_{SIF,PSII}$ is the contribution of PSII to the total SIF emission, f_{esc} is the escape probability that SIF emitted by PSII reaches the top of the canopy, determined as the ratio of NIR from vegetation to the fraction of incident PAR absorbed by the canopy (Zeng et al., 2019), and f_{λ} is the integration factor for the broadband SIF emission.

In addition to the FloX tower, where the sensors were located at a 2-m height, leaf-level measurements were also carried out. Using a LICOR LI-6400 device and a LI-

6400-40 fluorescence chamber, measurements of active fluorescence and gas exchange were taken. Based on this, it was possible to determine fluorescence characteristics including the contribution of PSII to the total SIF leaf emission $f_{\text{SIF,PSII}}$ and the maximum photochemical quantum yield $\Phi_{\text{PSII,max}}$. Please refer to Beauclaire et al. (2024a) for any additional information on the measurement campaign and data procedure.

2.2. Mechanistic light response (MLR) approach

2.2.1. Theoretical background

According to the work of Gu et al. (2019), the electron transport rate J_{SIF} is proportional to the fluorescence emitted by the PSII (SIF_{TOT}):

$$J_{\text{SIF}} = \frac{q_L \cdot \Phi_{\text{PSII,max}} (1 + k_{DF})}{1 - \Phi_{\text{PSII,max}}} \text{SIF}_{\text{TOT}} \quad (5.2)$$

where q_L is the fraction of open PSII reaction centers, $\Phi_{\text{PSII,max}}$ is the maximum photochemical quantum yield of PSII, determined by leaf-level measurements, and k_{DF} is the ratio, equal to a fixed value of 19 (Gu et al., 2019), between k_D and k_F , which are the rates of, respectively, the constitutive heat thermal dissipation and the fluorescence emissions. Based on Chang et al. (2021), q_L can be expressed as an exponential function of PAR and characterised by three empirical parameters:

$$q_L = a_{q_L} \cdot e^{-b_{q_L} \text{PAR}} + c_{q_L} \quad (5.3)$$

In the FvCB model, the net assimilation results from the comparison between A_v , known as the Rubisco-limited photosynthesis, and A_j the RuBP regeneration-limited photosynthesis (Chapter 2). GPP is thus dependent on the slower process between these two limiting rates. Conversely, in this current approach, it is assumed that J_{SIF} is a sufficient proxy for the dominant limitation, whether it is by RuBP regeneration, Rubisco or even triose phosphate utilisation (TPU), which is not considered in this version of the FvCB model. GPP can therefore be computed as follows:

$$\text{GPP}_{\text{SIF}} = J_{\text{SIF}} \frac{C_i - \Gamma^*}{4(C_i + 2\Gamma^*)} \quad (5.4)$$

where C_i is the CO_2 concentration in the leaf intercellular airspace, neglecting the mesophyll resistance, and Γ^* is the CO_2 compensation point, obtained with the leaf temperature as in the FvCB model. As a consequence, there is no longer need to compare the limiting rates, which stems from the fact that Equation (5.4) is valid regardless of the limitations when the *real* transport rate J is known (Harley et al., 1992). J is dependent on the irradiance, but also on the CO_2 partial pressure when Rubisco or TPU limits photosynthesis (Gu and Sun, 2014). Although the FvCB model differentiates between actual and potential J , it assumes a constant J with changes in CO_2 partial pressure, making the comparison between limiting rates compulsory in this method.

2.2.2. Integration into Daisy

In Daisy, the FvCB model is constructed as a layered two-leaf model. It means that the whole canopy is divided vertically in layers of equivalent leaf area index (LAI). In each layer, photosynthesis is computed for the sunlit and shaded leaves separately. To do so, the PAR absorbed by the canopy is distributed between each layer as well as each leaf fraction (sunlit or shaded) as described in de Pury and Farquhar (1997).

In their recent work, Chen et al. (2024b) estimated GPP_{SIF} for various canopy structures (layered and/or two-leaf). For the layered two-leaf construction, they partitioned SIF_{TOT} between each layer and leaf fraction following the absorbed PAR distribution. As a result, the SIF emitted by sunlit leaves in the layer i is expressed as:

$$SIF_{sun,i} = \frac{aPAR_{sun,i} \cdot \Phi_{Fsun,i}}{\sum_{k=1}^n aPAR_{sun,k} \cdot \Phi_{Fsun,k} + \sum_{k=1}^n aPAR_{shd,k} \cdot \Phi_{Fshd,k}} SIF_{TOT} \quad (5.5)$$

where n is the number of LAI layers in the canopy, $aPAR$ is the absorbed PAR and Φ_F is the fluorescence quantum yield which can be measured with the leaf fluorescence chamber. Chen et al. (2024b) found that having different Φ_F for sunlit and shaded leaves did not significantly impact the results. Additionally, we assumed that the vertical distribution of Φ_F was homogeneous as well, as winter wheat crops have relatively simple canopy compared to forests. Therefore, Equation (5.5) became:

$$SIF_{sun,i} = \frac{aPAR_{sun,i}}{\sum_{k=1}^n aPAR_{sun,k} + \sum_{k=1}^n aPAR_{shd,k}} SIF_{TOT} \quad (5.6)$$

This equation is also valid for shaded leaves, provided that the subscripts *sun* and *shd* are switched. GPP_{sun} and GPP_{shd} are computed over the entire canopy using respectively SIF_{sun} and SIF_{shd} instead of SIF_{TOT} in Equation (5.2), and ultimately summed to get the total GPP_{SIF} . As a result, GPP_{SIF} only depends on SIF_{TOT} given as input and on C_i . This equation is coupled with the stomatal conductance model from Leuning (1995) and adjusted to drought stress by Plauborg et al. (2010), allowing to estimate both GPP_{SIF} and C_i using Newton-Raphson method. In this current implementation, parameters are $\Phi_{PSII,max}$, set to 0.81 (Beauclaire et al., 2024a), as well as a_{qL} , b_{qL} and c_{qL} that need to be calibrated.

Because SIF measurements are restricted to a 10–17h window and data gaps within this window cannot be filled as easily as meteorological data, there were time steps without SIF measurements as model input. On those occurrences, the photosynthesis was simulated with the FvCB model instead of the MLR model.

2.3. Multi-objective calibration

Using the MLR approach, FvCB parameters previously calibrated in Chapter 4 (fP-SII and Xn) are no longer needed. Nevertheless, the other parameters from Table 4.2 are still required to run Daisy, in addition to the three newly integrated q_L parameters. As this chapter focuses on the integration of a SIF-based photosynthesis model, we only considered a_{qL} , b_{qL} and c_{qL} as targeted parameters for calibration. The other parameters were retrieved from the parameter set minimising F_{NEE} in Chapter 4 (Figure 4.1, also highlighted in green in Figure 5.6). These parameter values, or ranges if calibration is needed, are summarised in Table 5.1.

As in Chapter 4, we employed the Speed-constrained Multi-objective Particle Swarm Optimisation (SMP SO) algorithm for this multi-objective calibration. This algorithm generated parameter sets, specifically sets of three parameters in this case. Daisy was executed with these potential solutions, and the relative RMSE was computed for dry matter (DM), NEE and LE. Compared to Chapter 4, we only simulated S22 (i.e., winter wheat 2021-2022) since SIF measurements were available only for this season.

Table 5.1: Daisy parameters: values or calibration ranges (from measurements and literature).

Parameter	Value	Units	Description
a_{qL}	0.1-1	-	Exponential q_L parameter
b_{qL}	0.0005-0.005	-	Exponential q_L parameter
c_{qL}	0-0.45	-	Exponential q_L parameter
D ₀	2820	Pa	Leuning empirical coefficient
g ₁	16.79	-	Leuning stomatal slope
g ₀	0.01324	mol m ⁻² s ⁻¹	Leuning stomatal intercept
δ	0.8232	-	Empirical constant for hydraulic signalling
SpLAI	0.01522	m ² g ⁻¹	Specific leaf area
ShldResC	42.54	%	Capacity of reserves as fraction of stem DM
NII _{crit}	1.346	-	Stem/leaf partitioning modifier (threshold)
SOrgPhotEff	0.6703	-	Photosynthetic efficiency of storage organ
StemPhotEff	0.7606	-	Photosynthetic efficiency of stem
PenPar2	4.822	°C	Root penetration rate parameter (threshold)
σ _{NIR}	0.8926	-	Leaf scattering coefficient of NIR
ε _{leaf}	0.9825	-	Leaf emissivity for longwave radiation
k _{net}	0.3572	-	Radiation extinction coefficient
A _{brunt}	0.5548	-	Brunt parameter (offset)
B _{brunt}	0.06806	hPa ^{-1/2}	Brunt parameter (vapour pressure factor)
K _e	0.4724	-	Conversion of ET ₀ to bare soil evaporation
K _c	1.106	-	Conversion of ET ₀ to crop transpiration
K _{sat,1}	0.0452	cm h ⁻¹	Hydraulic conductivity at saturation (1 st layer)
K _{aquitard}	0.03667	cm h ⁻¹	Hydraulic conductivity at saturation (aquitard)
Z _{aquitard}	1.974	m	Thickness of the aquitard

3. Results

3.1. Pareto front

The 3D Pareto front depicted in Figure 5.1 is mostly driven by the trade-off between NEE and DM, whereas the front between NEE and LE is not clearly defined. Compared to F_{NEE} , the range of F_{DM} and F_{LE} are much narrower. This is expected as only q_L parameters were calibrated and they have a direct impact on photosynthesis. On the other hand, the other parameters (non-photosynthetic) were not calibrated but determined using the NEE-optimised solution from Chapter 4 (as detailed in Table 5.1), so the variations for each objective stem only from variations in photosynthesis.

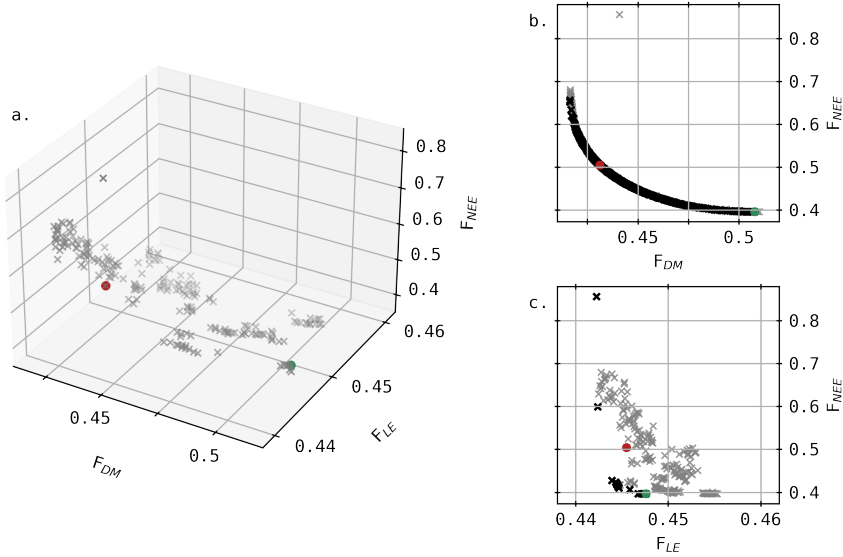


Figure 5.1: Non-dominated solutions in the objective space: (a) 3D and (b, c) 2D Pareto fronts according to the rRMSE of DM, LE and NEE. The red point highlights the most balanced compromise and the green point indicates the NEE-optimised solution.

It is worth noting that, even if the parallel can be drawn between Figure 4.1 and Figure 5.1, with a predominant trade-off between NEE and DM, these figures do not represent the exact same data. Values of rRMSE depicted in Figure 4.1 encompass four growing seasons of winter wheat whereas only one season (S22) is considered in

Figure 5.1. If the results using the FvCB model would only include S22, F_{DM} would range from 0.145 to 0.591, F_{NEE} from 0.320 to 0.628 and F_{LE} from 0.410 to 0.497. This can explain why higher values of F_{DM} and lower values of F_{NEE} and F_{LE} are observed in Figure 5.1, compared to Figure 4.1.

In the following sections, outputs simulated with the MLR and FvCB models are compared and discussed. These simulations were both based on the NEE-optimised parameter set, represented by the green point in, respectively, Figures 5.1 and 5.6 (in the appendices).

3.2. NEE fluxes

In Figure 5.2, NEE is simulated using the FvCB photosynthesis model in orange or, when there are SIF measurements, using the MLR model in purple. Daily evolutions are depicted in Figure 5.2a, with grey periods indicating when SIF was available, and hourly comparisons between predictions and observation are plotted in Figure 5.2b only when SIF was actually measured. As a reminder, when SIF was not available, the FvCB model was used even for the purple simulation. Consequently, days without SIF measurements show similar results in Figure 5.2a and, on the other days, the observed differences between MLR and FvCB might be partly muted as these measurements are restricted to a time window of 10-17h.

Regardless of the photosynthesis model used, both accurately captured the seasonal evolution of NEE. However, both also failed to predict NEE during the grain filling period (late June until harvest). As the crop is yellowing and ripening, both models expected a reduced photosynthesis. Nevertheless, photosynthesis was limited too much and was thus underestimated during this period, which is in accordance with the underestimation of crop yield observed in the previous chapter (Figure 4.2).

Major daily differences between FvCB and MLR occur around stem elongation (mid April to mid May) and grain filling (late June to early July). In April, NEE simulated with MLR is higher (i.e., closer to zero) until the 20th before reaching much lower values than with FvCB. This transition coincides with a sudden increase of f_{esc} (+60% from 20 to 23 April), meaning that there is more green leaf surface within the canopy. Around stem elongation, the largest differences between FvCB and MLR occur on 3 and 4 May, which are represented by the lowest purple points in Figure 5.2b. From late June to early July, NEE simulated with MLR is higher than with FvCB (Figure 5.2a) and corresponds to the highest purple points in Figure 5.2b, i.e. the cloud of points where predictions are mostly positive but observations negative. Measurements of SIF_{TOC} around this period are close to zero, specifically ranging from 0.016 to 0.23 $\mu\text{mol m}^{-2} \text{s}^{-1}$. Therefore, $|GPP_{SIF}|$ is low as well, explaining that NEE predictions can be positive. Nevertheless, these few summer days highly contribute to the RMSE, as this metric falls from 5.82 to 4.19 $\mu\text{mol m}^{-2} \text{s}^{-1}$ when they are not included in the calculation.

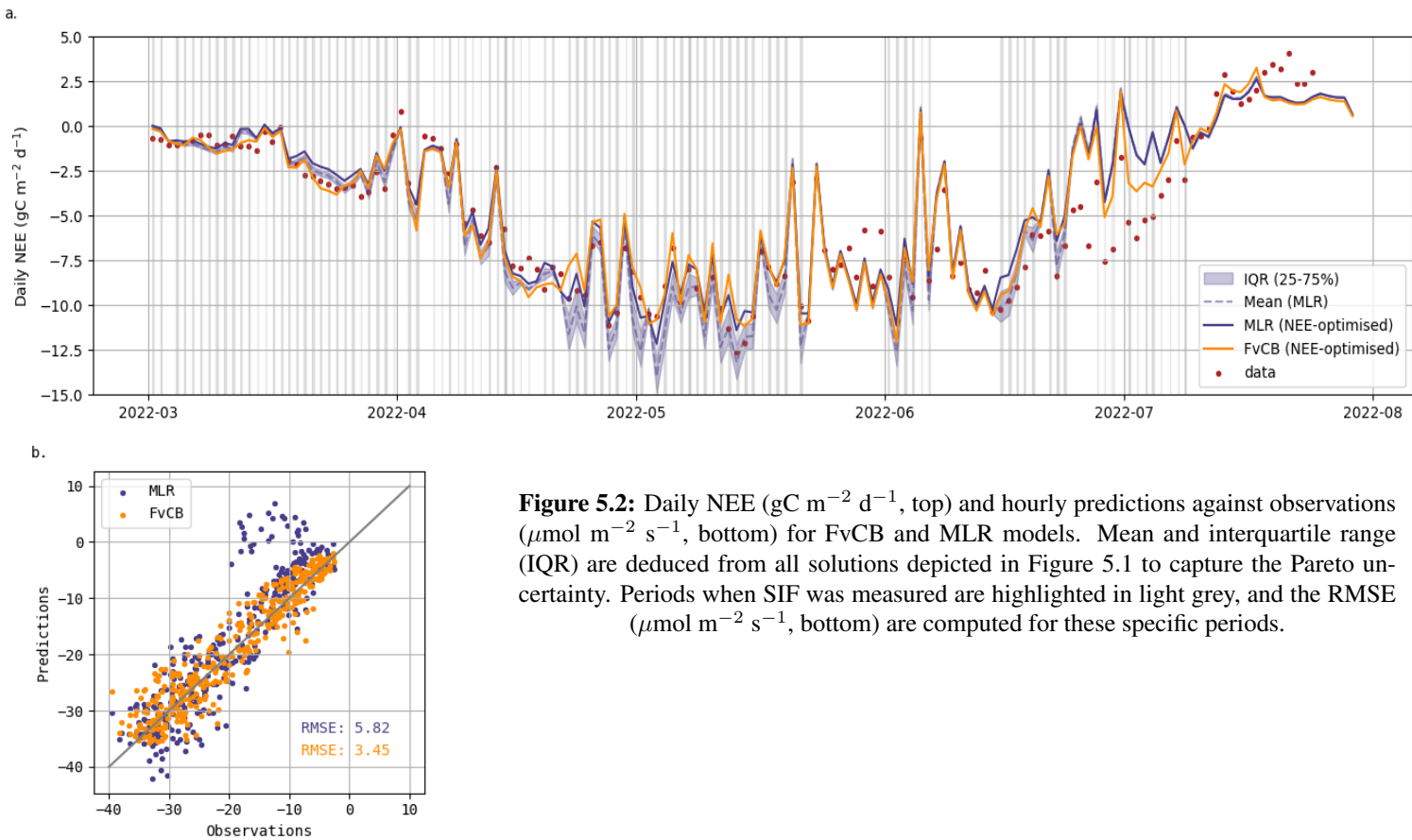


Figure 5.2: Daily NEE ($\text{gC m}^{-2} \text{d}^{-1}$, top) and hourly predictions against observations ($\mu\text{mol m}^{-2} \text{s}^{-1}$, bottom) for FvCB and MLR models. Mean and interquartile range (IQR) are deduced from all solutions depicted in Figure 5.1 to capture the Pareto uncertainty. Periods when SIF was measured are highlighted in light grey, and the RMSE ($\mu\text{mol m}^{-2} \text{s}^{-1}$, bottom) are computed for these specific periods.

3.3. *NEE residuals*

Residuals plots show the difference between predicted and observed NEE as a function of a given variable. To enable fair comparison between the equivalent residuals plots, we only kept data when SIF was measured, even for the FvCB model. As mentioned previously, these measurements are taken between 10 and 17h when NEE is mainly driven by GPP. As GPP is considered to be negative, positive residuals mean that predicted GPP is underestimated, or vice-versa. Furthermore, we discarded data from 27 June to harvest, this period is extensively discussed in Section 4.2.3.

3.3.1. FvCB model

Using the FvCB model, NEE residuals have only a strong dependence on incoming global radiation and, more specifically, its diffuse fraction (Figure 5.3). This photosynthesis model tends to underestimate GPP when the incoming global radiation is low and diffuse. Conversely, predicted GPP is typically overestimated if radiation has a small diffuse fraction. These two dependences are also observed when all data are included (i.e., whether there are SIF measurements or not), with a stronger dependence on the diffuse fraction ($p = 8 \cdot 10^{-55}$). In Figure 5.3, the biggest overestimations are observed on 14 March and 12 April, both being around $-10 \mu\text{mol m}^{-2} \text{s}^{-1}$. Compared to the other surrounding days, the photosynthesis observed on those days appears to be limited by one or several factors not considered in the FvCB model.

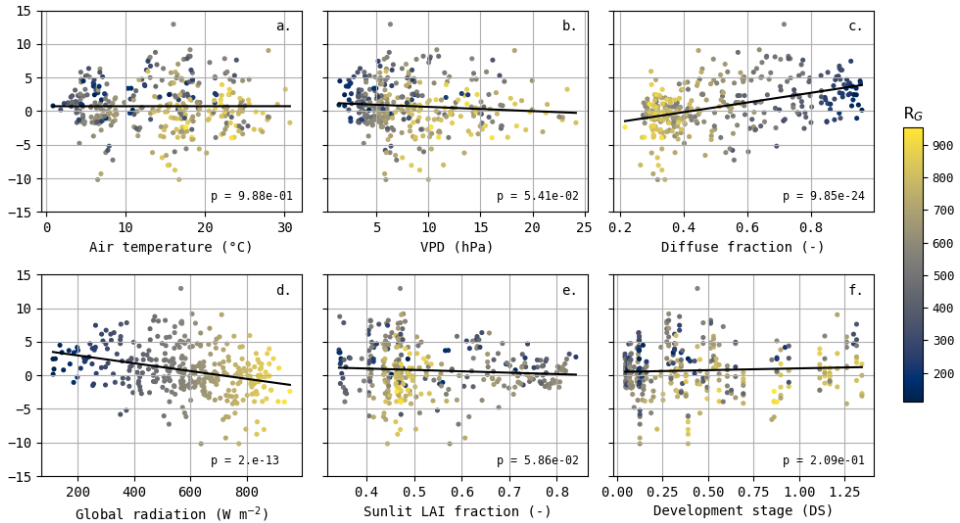


Figure 5.3: NEE Residual plots (FvCB predictions minus observations, $\mu\text{mol m}^{-2} \text{s}^{-1}$) according to environmental and crop variables. Residual mean ($\pm\sigma$) is equal to $0.274 \pm 3.46 \mu\text{mol m}^{-2} \text{s}^{-1}$. The p-value indicates if the linear regression slope is significantly different from 0 and the colour of the points depends on the incoming global radiation.

Slope value of each plot is available in the appendices (Table 5.2).

3.3.2. MLR model

With the MLR model, the dependence of the residuals on global radiation and its diffuse fraction is reduced, especially for the diffuse fraction, but other dependences arise such as SIF_{TOC} , f_{esc} , SIF_{TOT} as well as the sunlit LAI fraction (Figure 5.4). The MLR model underestimates crop photosynthesis when the fluorescence and radiation are low and when the sunlit LAI fraction is high. The strong influence of SIF_{TOC} , SIF_{TOT} and f_{esc} can indicate shortcomings in the relationship between GPP and SIF or in the process of acquiring and handling SIF data itself. As for the dependence on sunlit LAI fraction, this dependence raises questions about the differences in behaviour between sunlit and shaded leaves.

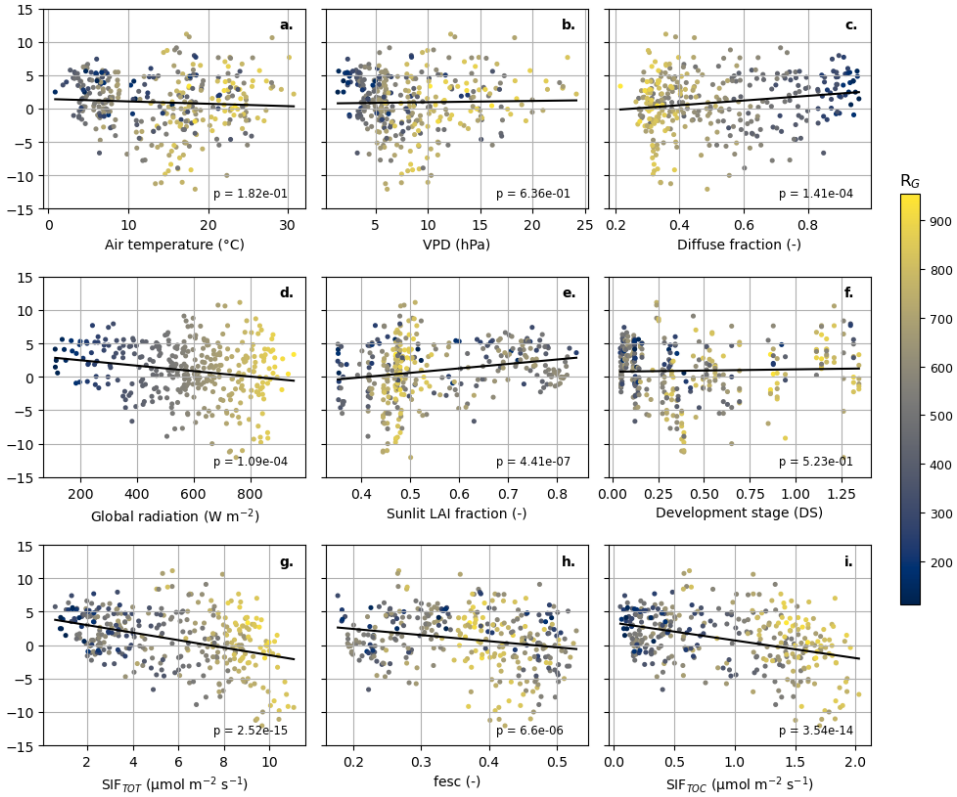


Figure 5.4: NEE Residual plots (MLR predictions minus observations, $\mu\text{mol m}^{-2} \text{s}^{-1}$) according to environmental and crop variables. Residual mean ($\pm\sigma$) is equal to $0.924 \pm 4.12 \mu\text{mol m}^{-2} \text{s}^{-1}$. The p-value indicates if the linear regression slope is significantly different from 0 and the colour of the points depends on the incoming global radiation.

Slope value of each plot is available in the appendices (Table 5.2).

4. Discussion

Using the FvCB model, Daisy already had proven ability to accurately capture the daily and hourly evolution of NEE and, to a lesser extent, LE (Chapter 4). With this new approach, using the MLR model, we found RMSE values of $5.82 \mu\text{mol m}^{-2} \text{s}^{-1}$ (Figure 5.2b) and 66.8 W m^{-2} (Figure 5.7) for NEE and LE respectively. As a comparison, using the same dataset, the RMSE values were equal to $3.45 \mu\text{mol m}^{-2} \text{s}^{-1}$ and 57.8 W m^{-2} with FvCB, meaning that both NEE and LE were better predicted using FvCB than MLR. However, regardless of the model used, GPP is underestimated during the grain filling period, when newly assimilates are allocated to the storage organs, leading to an underestimation of crop yield.

Furthermore, as depicted in Figure 5.1, the trade-off between DM and NEE is even more exacerbated when using MLR, compared to Figure 4.1. The integration of a SIF-based photosynthesis model did not improve the simultaneous simulation of DM and NEE. The possible explanations for this trade-off have already been explored in Chapter 4 and should continue to be tested. Additionally, it would be worth applying the SMPSO algorithm when considering all parameters listed in Table 5.1 as targeted parameters. It would allow to verify whether the front in Figure 5.1 is accentuated because only photosynthetic q_L parameters were calibrated and check the shape of the front between NEE and LE. Similarly, fixing the stomatal parameter δ to 0 would also be interesting. In the current implementation, drought can have a two-fold effect: stomatal conductance is reduced by hydraulic signalling and photosynthesis is impacted through SIF changes. Hence, drought response might currently be exaggerated. Despite these noteworthy points that still need to be further analysed, the comparison between the photosynthesis models allowed us to identify advantages and limitations in both of them.

4.1. What are the limitations of the FvCB model?

4.1.1. Considering light quantity but not quality

The FvCB model traditionally treats all PAR (400-700 nm) as equivalent in terms of its efficiency in driving photosynthesis. However, the leaf absorbance and quantum yield of photosynthesis differs between wavelengths (Liu and Van Iersel, 2021). Green light is less absorbed by the leaves than red and blue light. As a consequence, incident red and blue light have a higher quantum yield of photosynthesis. Nevertheless, under high intensity, green light can have greater quantum yield because it can penetrate deeper in cell layers, reaching further photosystems while red and blue light

are restricted to the outer layers (Terashima et al., 2009; Liu and Van Iersel, 2021). To take this analysis a step further, and even if red and blue light have similar absorption coefficients in leaves, they can produce various physiological responses:

- **Stomatal aperture.** Stomata are known to respond to light in two ways. First, the quantitative (or 'red' light) response relies more on the quantity of incident light than on its spectral composition. Second, at equivalent light quantity, stomata would open wider when induced by blue light specifically, due to photoreceptors called phototropins (Kromdijk et al., 2019).
- **PSI/PSII excitation balance.** Photosystem I (PSI) is preferentially excited by red and far-red light whereas PSII is rather excited by wavelengths ranging from 450 to 680 nm (Jans et al., 2025). Depending on the incident light spectrum, leaves can thus be in a PSI/PSII imbalance state which ultimately impacts photosynthesis (Taylor et al., 2019).
- **PAR quanta-to-energy ratio.** PAR can be expressed in energy units (W m^{-2}), describing the energy it carries, or in quantum units ($\mu\text{mol m}^{-2} \text{s}^{-1}$) which is the photosynthetic photon flux density (PPFD). The conversion between these two units depends on the spectral composition of light (Möttus et al., 2012; Dye, 2004).

All these factors are not considered in the FvCB model and could explain the strong dependences of NEE residuals observed in Figure 5.3c, d. When the diffuse fraction is high, the blue-to-green and blue-to-red ratios are higher. As a consequence, stomata may actually open more than predicted which finally leads to an underestimation of photosynthesis. However, blue-enriched spectra carries fewer photons per unit of energy, as the quanta-to-energy ratio is smaller. Therefore, as Daisy uses a fixed conversion ratio, based on McCree (1972), to estimate PPFD from global radiation, PPFD and hence photosynthesis may be overestimated. These opposing arguments make the interpretation of the results challenging. This difficulty is reinforced by the effect of blue light on PSI/PSII balance. While blue light overexcites PSII relatively to PSI, limiting linear electron transport, this imbalance can be partially compensated by state transitions (Taylor et al., 2019; Rochaix, 2014). This is a short-term regulatory mechanism where light-harvesting complex II antenna can migrate between photosystems (Rochaix, 2014).

To better understand each implication, it would be best to integrate these mechanisms into photosynthesis models. Although difficult, this task has been eased by the recent advances and expansion of optical measurements. Lately, Jans et al. (2025) proposed a modified FvCB model to account for PAR spectrum as well as far-red (380 to 780 nm). In their wavelength-dependent model, they also considered the distinct excitation of PSI and PSII by this incident light. Similarly, Kromdijk et al. (2019)

expressed the stomatal conductance as a function of light, with $1 - q_L$, rather than net assimilation. This formulation, including the light response of stomata, produced equally good predictions compared to Ball-Berry stomatal model while decreasing the modelling complexity.

4.1.2. Other limitations

Although not related to the diffuse fraction of incoming light, few other limitations of the FvCB model have been reported and analysed, and may contribute to the observed RMSE of $3.45 \mu\text{mol m}^{-2} \text{s}^{-1}$ (Figure 5.2). These include the missing limitation by triose phosphate utilisation, the omission of the mesophyll resistance, the dynamic evolution of NPQ, the lacking effects of photoinhibition and the steady-state assumption (Yin et al., 2021; Bambach et al., 2020; Morales et al., 2018).

The triose phosphate utilisation (TPU) limitation rate is defined in the initial version of the FvCB model (Farquhar et al., 1980) but is often dropped in model implementations like in Daisy (Gregory et al., 2021). TPU represents the conversion of triose phosphates into other sugars, mostly starch and sucrose and is known to limit photosynthesis at high CO_2 and incident radiation. This TPU-limited photosynthesis becomes insensitive to CO_2 and even declines with increasing CO_2 but becomes more sensitive to temperature (Yang et al., 2016a). As shown in Figure 5.3d, GPP predicted by the FvCB model is overestimated under high incoming radiation. It would be valuable to integrate this third limiting rate to check if the discrepancies are partly due to a missing photosynthesis limitation.

As already discussed in Chapters 3 and 4, the mesophyll conductance is considered to be infinite in FvCB, assuming that CO_2 concentration in the intercellular airspaces is identical in the chloroplasts. However, this conductance seems to significantly impact photosynthesis as well as its coupling with transpiration, especially under water-stressed conditions (Nadal and Flexas, 2018). Slowly but surely, its parameterisation is implemented into more models such as the terrestrial biosphere model JSBACH (Knauer et al., 2020).

Photoprotection is a set of plant mechanisms that occur when plants absorb more energy than they can use, and which includes NPQ, state transitions and photoinhibition. Under excessive light, NPQ is a momentary downregulation of maximum quantum yield of PSII $\Phi_{\text{PSII,max}}$, resulting in a reduction of photosynthesis and an increase in heat dissipation (Murchie and Ruban, 2020). Compared to NPQ, which is a protective and rapidly reversible mechanism, photoinhibition induces physiological damages and it takes hours to days for $\Phi_{\text{PSII,max}}$ to recover. In contrast to MLR, these mechanisms are not taken into account in the FvCB model as $\Phi_{\text{PSII,max}}$, which is implicitly included in f_{PSII} parameter (Long and Bernacchi, 2003), is considered to be fixed.

As a steady-state model, FvCB describes photosynthesis when all processes have reached equilibrium with the environment conditions. However, leaves are subject

to continuous light fluctuations, mainly due to diurnal sun angle changes, sunflecks, intermittent cloud cover and wind-driven leaf movement (Wang, 2024; Pearcy et al., 2004). On the other hand, the plant responses to these dynamic variations can be much slower, requiring for instance about 15 min to regain maximum photosynthetic efficiency when going from shade to sun conditions (Taylor and Long, 2017). Each process affected by variations in incident radiation have its own response time, not to mention the time for stomatal opening, Rubisco (de)activation or NPQ induction and relaxation. As a consequence, the instantaneous rate of photosynthesis can deviate substantially from steady-state predictions (Wang et al., 2020).

4.2. *Is the MLR model the right answer?*

Compared to the FvCB model, photosynthesis modelling with the MLR model is slightly more straightforward, with fewer parameters (e.g., no Michaelis-Menten kinetics, no $V_{c,max}$) and a real estimation of the actual electron transport rate. Photosynthesis, along with C_i , still needs to be estimated numerically using Newton Raphson method, so the gain in computing time is negligible. The main difference comes from the inputs required to run the model. The MLR model heavily relies on the SIF measurements which implicitly include some mechanisms missing in the FvCB model, such as the photoprotection or the implicit stomatal response to light. However, this also makes the MLR model highly dependent on the data coverage and treatment. Highlighted in grey in Figure 5.2, periods when SIF was measured accounted for 22.45% of the entire calibration period. This percentage would more or less double when considering only periods during daytime, when crops actually photosynthesise. While gap-filling methods are increasingly developed and used for satellite products (Li et al., 2026; Verrelst, 2026; Tadić et al., 2024), only few attempts were made for SIF from ground instruments (Biriukova et al., 2021). Due to its fine temporal resolution and spatial location, *in situ* SIF serves as gap-filling or validation data for satellite products, rather than the opposite. However, growing attention is being paid to SIF data as a whole and further developments are expected, particularly given the recent Fluorescence Explorer (FLEX) mission (Verrelst, 2026).

Besides the data coverage, NEE residuals show significant dependences on SIF_{TOT} , f_{esc} and SIF_{TOC} as depicted in Figure 5.4g-i. It suggests that (i) systematic errors exist within the multi-step procedure for estimating SIF_{TOT} , which is discussed in Section 4.2.1, or (ii) the MLR formalism does not fully capture the information contained in the SIF signal, discussed in Section 4.2.2.

4.2.1. Challenges in estimating SIF_{TOT}

As explained in Section 2.1, it is possible to determine SIF_{TOT} based on only two continuous measurements: the downwelling solar irradiance and upwelling radiance. Nevertheless, this estimation contains multiple challenges and strong assumptions (Porcar-Castell et al., 2021) that may partly explain the obtained results.

The first step, which consists of separating SIF from the true reflectance of the canopy, is called **SIF retrieval** and is conducted using the SFM. Compared to the Fraunhofer lines discriminator (FLD), which requires spectrometers with high spectral resolution as well as longer periods of signal integration (Porcar-Castell et al., 2021), SFM is more sensitive to atmospheric absorption and scattering of SIF. In this study, it was assumed that, as the sensors are close to the canopy, the atmospheric path can be neglected and that measurements are acquired at the same height as the canopy. However, throughout the cropping season, this distance has changed, ranging from 1.2 m in June to 1.9 m in March. According to Sabater et al. (2018), a distance of even a few meters between the sensors and the canopy could result in significant errors, and contribute to dependence depicted in Figure 5.4i. This first challenge is depicted on the right-hand side of Figure 5.5, where retrieved SIF_{TOC} in light red might be different from SIF escaping from canopy due to atmospheric attenuation. The greatest attenuation is illustrated around 760 nm, which corresponds to the $\text{O}_2\text{-A}$ absorption band used in this study.

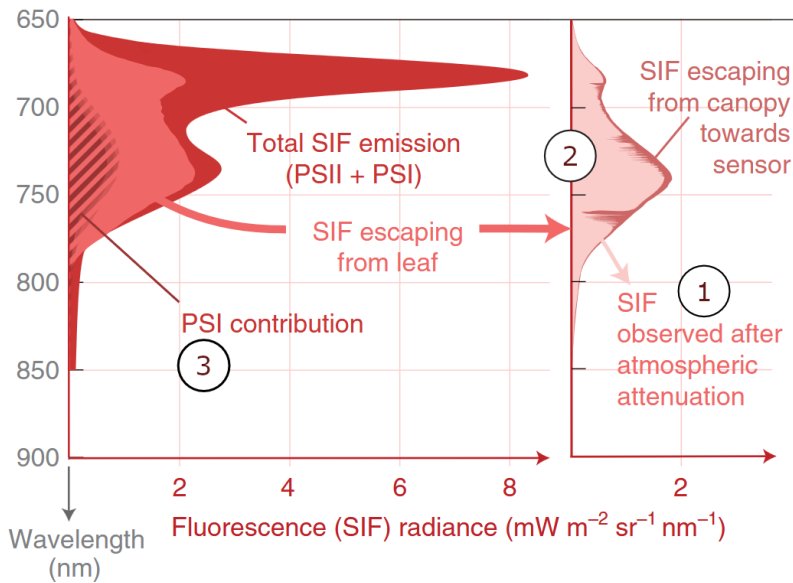


Figure 5.5: Challenges in estimating SIF_{TOT} from radiance measurements, adapted from Porcar-Castell et al. (2021). On the left-hand side, total SIF emission by the photosystems is depicted in dark red, with the PSI contribution explicitly indicated. Total SIF emission escaping the leaves, in light red, is smaller as photons can be reabsorbed within the leaves. Same goes for the SIF escaping from canopy, in dark red on the right-hand side, as photons can be reabsorbed and scattered within the canopy.

Once SIF_{TOC} is estimated from hyperspectral measurements, the broadband SIF emitted by PSII can be found using Equation (5.1). When emitted by leaves, SIF might be scattered or reabsorbed within the leaves and canopy before reaching the top

of the canopy. This is characterised by f_{esc} , representing the **escape probability** that emitted SIF reaches the top of the canopy. Based on the formulation proposed by Zeng et al. (2019), f_{esc} is taken as the ratio between NIR_v , a vegetation index based on NIR reflectance (Badgley et al., 2017), and the fraction of incident PAR absorbed by the canopy (fAPAR). However, this escape probability is known to depend on spatial and temporal variations in canopy architecture as well as in leaf biochemistry and morphology (Porcar-Castell et al., 2021). This simplified method of Zeng et al. (2019) assumes homogeneous canopy layers, contrary to much more complex radiative transfer models such as SCOPE or DART (Van Der Tol et al., 2009; Yang et al., 2017; Gastellu-Etchegorry et al., 2017). These assumptions could explain the observed dependence on f_{esc} (Figure 5.4h). In Figure 5.5, this second challenge is depicted by the difference between the SIF in darker red on the left and in darker red on the right.

The third challenge is the partitioning of total SIF emissions between photosystems (PSI and PSII). While the sensor does not differentiate between SIF emitted by PSI or PSII, the MLR model requires only the **contribution of PSII**. In Equation (5.1), this is defined by $f_{SIF,PSII}$ which is determined by leaf-level fluorescence measurements under specific light quality (Beauclaire et al., 2024a). In the literature, the contribution of each photosystem, as well as the distribution of excitation energy between them, are known to vary over time, but the driving variables are still under research (Porcar-Castell et al., 2021; Guo et al., 2024). The mostly known driver for $f_{SIF,PSII}$ is the light intensity (Guo et al., 2024; Guo et al., 2025), which is also the case for this growing season as it varied linearly between 0.55 and 0.75 as a function of light intensity (Beauclaire et al., 2024a). As shown in Figure 5.4, diffuse fraction of incoming radiation still has a significant impact on NEE residuals. How $f_{SIF,PSII}$ responds to different excitation wavelengths remains an open question that warrants further investigation.

4.2.2. Linking GPP to SIF_{TOT}

With SIF_{TOT}, the SIF emitted by PSII, it is then possible to estimate GPP_{SIF} using Equations (5.2) to (5.6). However, these relationships also rely on strong assumptions that need to be discussed and for which alternative formalisms exist or are currently studied.

As a reminder, the **fluorescence quantum yield** Φ_F represents the ratio of the fluorescence emission rate to the sum of all rates (PQ, NPQ and F). This ratio changes depending on environmental conditions, reflecting the PQ and NPQ dynamics (Porcar-Castell et al., 2021). Based on Chen et al. (2024b), we considered an identical Φ_F for sunlit and shaded leaves, even though it was found that leaves adjusted their photosystem stoichiometry according to their status (Hogewoning et al., 2012). For instance, under a shade light spectrum (far-red), leaves would reduce the relative amount of PSI to counter its overexcitation. Besides this response, temperature also influences the three rates (PQ, NPQ and F) and should have been taken into account (Xia et al., 2018; Groot et al., 1994). Although not considered in Chen et al. (2024b), shaded and sun-

lit leaves can have different temperatures. During S22, sunlit leaves were estimated to be 0.58°C hotter than shaded leaves on average, with a simulated maximal difference of 5.27°C . Including these influences could have reduced the dependence of NEE residuals on global radiation and sunlit LAI fraction (Figure 5.4d,e).

The second assumption comes from the **estimation of the fraction of open PSII reaction centres** q_L . This factor plays a crucial role in the MLR model, as it is proportional to J_{SIF} in Equation (5.2). These open PSII reaction centres become oxidised while transferring electrons to plastoquinone and thus transition to a closed state (Liu et al., 2024c). Therefore, as q_L was found to decrease with increasing PAR, it has been empirically linked to this radiative flux through an exponential function (Chang et al., 2021). This relationship has, however, been recently discussed, arguing that PAR is not the only predictor. For instance, Han et al. (2022) highlighted the role of temperature in q_L temporal variability. To address that, Liu et al. (2024c) expressed q_L as a function of SIF_{TOT} and leaf temperature. Using SIF_{TOT} instead of PAR aimed to include information of canopy structure in the estimation of q_L and no longer need PAR as input (Liu et al., 2024c). They reported better predictions of GPP, with a rRMSE of 12% compared to 18.8% using q_L -PAR relationship. Shortly after, Guo et al. (2025) further extended this new formalism with an adapted measurement design.

Finally, the **assumption of a steady coupling** between SIF and GPP, which underlies the MLR model, has been repeatedly questioned in the literature. Several studies have reported decouplings between SIF and GPP under specific environmental conditions. For instance, when stomata close under soil water stress, the photosynthetic rate decreases rapidly while SIF is relatively less affected, resulting in a decoupling between fluorescence and photosynthesis (Jia et al., 2023). Under heat stress, the decoupling can be even more pronounced. Martini et al. (2022) showed that the 2018 European heatwave caused an inversion of the photosynthesis–fluorescence relationship at both the canopy and leaf scales. The decoupling was strongly shaped by NPQ quantum yield, as excess excitation energy was dissipated as heat rather than fluorescence. Working on multiple biomes, Liu et al. (2022a) showed that the relationship between SIF and GPP at the canopy level varies widely, reflecting the role of canopy architecture at seasonal timescales. When relying on SIF as a direct proxy for GPP, it implicitly assumes a stable coupling between fluorescence emission and carbon assimilation, which may not hold across all growth stages or stress conditions.

A promising alternative to bridge the gap between fluorescence and photosynthesis modelling is the mechanistic framework proposed by Johnson and Berry (2021), centred on the cytochrome b_6f (Cb6f) complex. Instead of expressing J as an empirical function of PAR (Farquhar et al., 1980) or inferring it from SIF measurements (Gu et al., 2019), they assumed that Cb6f acts as the primary regulator of linear electron transport. In their formulation, Cb6f is seen as a transistor, operating at constant and maximum conductance under limiting light (i.e., when J is dependent on plastoquinol

PQH₂ supply and its oxidation rate by Cb6f) and switching to a variable and lower conductance under saturating light (i.e., when feedback from carbon metabolism downregulates Cb6f conductance). This approach offers a more physically based alternative as it explicitly models the Cb6f kinetics, the state of PSI/PSII reaction centres, NPQ heat dissipation, cyclic electron transport and the subsequent regulation of photosynthesis. Building on this framework, Guo et al. (2026) proposed a new practical approach to estimate the maximum activity of Cb6f from SIF observations. They demonstrated that the Cb6f model outperformed the standard FvCB model in estimating half-hourly GPP at a winter wheat site, with the main improvement coming from a better representation of shaded leaf photosynthesis. This suggests that incorporating Cb6f dynamics into canopy-scale photosynthesis models could constitute a valuable development.

4.2.3. What happened during the grain filling period?

As a reminder, a significant part of the RMSE calculated from NEE predictions and observations can be attributed to approximately twenty hours (Figure 5.2), all of which occurred during the grain filling period. During these hours, SIF measurements were close to zero, and consequently, predicted photosynthesis was also close to zero, whereas observations indicated substantially higher values.

After flowering, photosynthetic CO₂ fixation mainly occurs in flag leaves, sheath and ears, the latter composed of awns, glumes, paleas, lemmas and peduncles (Evans and Rawson, 1970; Tambussi et al., 2021). Compared to leaves, non-foliar organs have distinct photosynthetic properties such as photosynthetic rates, chlorophyll contents and $\Phi_{\text{PSII,max}}$ that are, moreover, changing over time (Wang et al., 2001). For instance, Kong et al. (2015) found that glumes have higher values of $\Phi_{\text{PSII,max}}$, experience higher NPQ and senesce later than flag leaves, revealing their substantial contribution to grain filling. Furthermore, because of the location and higher density of their stomata, non-foliar organs are more likely to re-fix respired CO₂ (Hu et al., 2019).

Consequently, using the MLR model during this period raises numerous questions. Do non-foliar organs emit more or less SIF compared to leaves? Is the decorrelation between SIF_{TOT} and GPP due to leaf-related parameters (i.e., leaf-level measurements $\Phi_{\text{PSII,max}}$ and $f_{\text{SIF,PSII}}$)? As non-foliar organs, located at the top of the canopy, have a much more complex morphology than leaves, how is the estimation of SIF_{TOT} impacted? In other words, scattering or reabsorption of emitted SIF might be different, should the escape probability f_{esc} be adapted to such situations and, if so, how?

These questions remain largely open and merit targeted future work. The grain filling period is a decisive phase for final grain yield, during which a substantial fraction of carbon assimilation occurs in non-foliar organs. Failing to represent this period accurately directly undermines the agronomic relevance of the model. Addressing this limitation will require dedicated organ-level fluorescence measurements during grain filling to consider the MLR model as a robust tool across the full winter wheat growing season.

5. Conclusion

Integrating the MLR model into Daisy is a first step toward incorporating SIF-based photosynthesis modelling into a process-based crop model, and the results open encouraging prospects for this approach. Despite the minimal calibration effort (only three q_L parameters) and the limited data coverage, the MLR model produced DM, NEE and LE simulations in the same range as FvCB, with RMSE values moderately higher. There is nevertheless room for improvement in the MLR approach, starting from the assumptions made in this study (e.g., constant Φ_F , q_L relationship) to the compounding uncertainties or biases introduced at each step of SIF_{TOT} estimation. Furthermore, although FvCB showed better results, both approaches underestimated photosynthesis during the grain filling period, pointing to a common structural weakness in representing non-foliar organ contributions. Future work should explore the cytochrome b_6f framework as a more physically grounded alternative to MLR and FvCB that also integrates SIF data, alongside dedicated fluorescence measurements on ears and flag leaves during grain filling.

6. Appendices

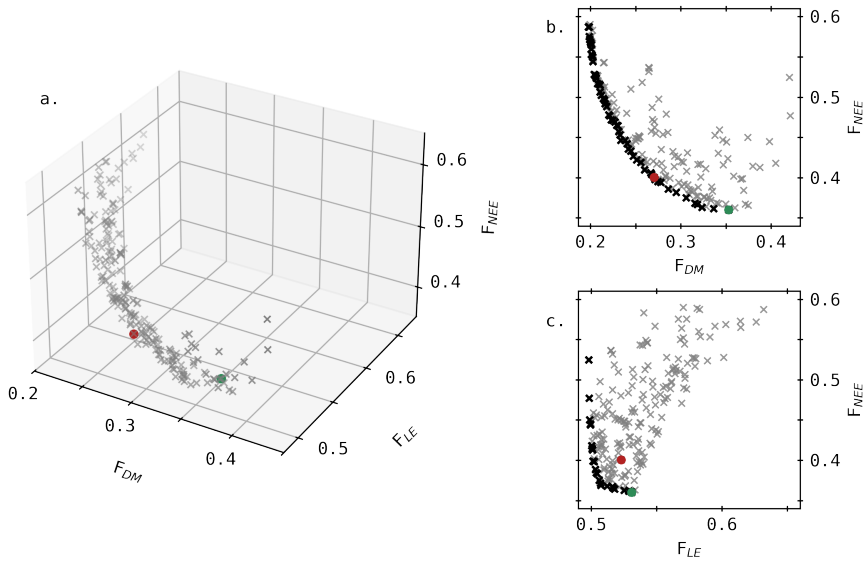


Figure 5.6: Non-dominated solutions in the objective space: (a) 3D and (b, c) 2D Pareto fronts according to the rRMSE of DM, LE and NEE. The red point highlights the most balanced compromise and the green point indicates the NEE-optimised solution.

Table 5.2: Slope and p-values of residual plots. The slope indicated by the superscript* is defined as the normalised slope, i.e. multiplied by the amplitude on the x-axis ($x_{\max} - x_{\min}$).

Variable	FvCB			MLR		
	Slope	Slope*	p-value	Slope	Slope*	p-value
Air temperature	3.43×10^{-4}	0.0103	0.988	-0.0355	-1.06	0.182
VPD	-0.0629	-1.43	0.0541	0.0193	0.440	0.639
Diffuse fraction	7.21	5.36	9.85×10^{-24}	3.49	2.60	1.41×10^{-4}
Global radiation	-0.00579	-4.88	2.00×10^{-13}	-0.00406	-3.42	1.09×10^{-4}
Sun LAI fraction	-2.06	-1.00	0.0586	6.68	3.25	4.41×10^{-7}
DS	0.534	0.695	0.209	0.352	0.458	0.523
SIF _{TOT}	-	-	-	-0.563	-5.89	2.52×10^{-15}
f_{esc}	-	-	-	-9.14	-3.22	6.60×10^{-6}
SIF _{TOC}	-	-	-	-2.64	-5.22	3.54×10^{-14}

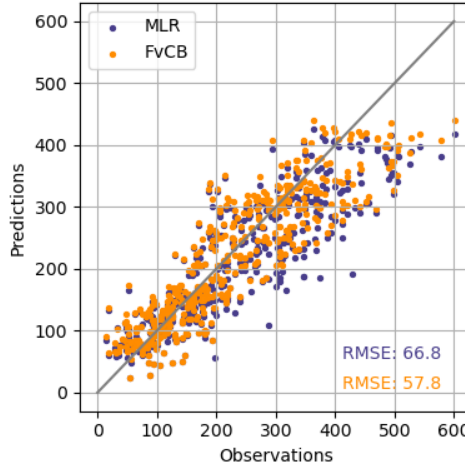


Figure 5.7: Hourly predictions against observations (W m^{-2}) for FvCB and MLR models. For each model, the RMSE (W m^{-2}) was computed only when SIF was measured.

6

Discussion and perspectives

1. Summary and discussion

1.1. Thesis overview

This thesis set out to model carbon, nitrogen, water and energy fluxes of winter wheat crops at the BE-Lon station, with the Daisy soil-plant-atmosphere model as the central modelling framework. Taken together, Chapters 3 to 5 constitute an integrated model assessment and development: sensitivity analysis informs calibration, calibration exposes structural weaknesses, and those weaknesses in turn motivate new process representations or targeted measurement campaigns. Rather than treating model and measurements as separate, each chapter highlights how the two can reinforce one another. Models reveal which measurements are most critical, while measurements constrain and challenge model structure. Hereafter, the main findings are synthesised through this lens before discussing important and suitable perspectives for future work.

Temporal GSA as a guide for measurement priorities. Chapter 3 demonstrated that temporal GSA provides substantially more information than aggregated approaches for understanding Daisy model behaviour. The temporal analysis revealed that parameter sensitivities are not constant over the growing season but undergo abrupt transitions associated with phenological stages and environmental conditions. With such an approach, modellers can identify the specific periods during which each parameter exerts the greatest influence and schedule a targeted field campaign accordingly. For instance, photosynthetic parameters (X_n , c_{vm} and f_{PSII}) dominated the variance of NEE and DM over much of the growing seasons, as expected, but it was also found that parameters characterising deep soil hydraulics can be as influential under specific meteorological conditions. The results of Chapter 3 indicate that uncertainties in $K_{sat,aq}$ and Z_{aq} , as well as in $K_{sat,4}$ and the horizontal-to-vertical anisotropy ratio, can propagate into major errors in simulated crop development during wet years. Compared to photosynthetic parameters that are more tightly constrained, these soil parameters have a large range of feasible values and are rarely measured *in situ*. Careful estimation should therefore be considered a priority for sites where the water table regularly rises into or near the root zone like in BE-Lon.

The diagnostic value of multi-objective calibration. Using SMPSO algorithm to simultaneously fit Daisy against DM, NEE and LE has proved to be particularly insightful. On the one hand, the strongly curved DM-NEE front suggests a conflicting trade-off between these two outputs, most likely arising from (i) an underestimation of heterotrophic respiration, (ii) wrong parameterisation of crop processes such as partitioning schemes or non-foliar photosynthesis, and (iii) possible biases in NEE measurements from EC systems. On the other hand, the nearly perpendicular LE-NEE

front is indicative of equifinality, probably due to the structural decoupling between soil evaporation E_{soil} and plant transpiration T_{plant} . However, EC systems measure NEE or LE fluxes as a single signal, hence NEE components (i.e., GPP and R_{eco}) and evaporation components (E_{soil} and T_{plant}) cannot be independently constrained. Without additional measurements, such as soil chambers or isotopic partitioning (Klosterhalfen et al., 2019), it is currently impossible to confirm any of the explanations reported in Chapter 4.

Promises and limits of SIF-based photosynthesis modelling. Chapter 5 explored the integration of SIF into Daisy via the MLR model. The rationale was compelling: because SIF is emitted as a by-product of PSII activity, it embeds ecophysiological information about light use and stress responses that is otherwise difficult to parameterise explicitly. Replacing the standard FvCB model with the MLR approach would therefore reduce the number of parameters requiring calibration while potentially yielding more realistic representations of photosynthesis under varying environmental conditions. Nevertheless, the MLR model did not outperform FvCB in simulating either NEE or LE. Besides the assumptions specific to the implemented MLR (e.g., constant Φ_F), the major constraints faced by this new approach are the data uncertainties and availability. To be successfully integrated into Daisy, the MLR model requires continuous high-quality SIF observations at each time step. However, the measurement window for SIF was restricted to 10–17h, during which data were also discarded due to unsuitable environmental conditions. Moreover, SIF is not measured directly but estimated from hyperspectral measurements, making it subject to compounding uncertainties extensively discussed in Section 4.2.1. In this sense, the SIF signal is simultaneously the most innovative input available at BE-Lon and the most constraining one.

1.2. How good is the abiotic stress simulated?

1.2.1. Waterlogged stress

Due to heavy rainfall in December 2014, the water table depth fluctuated between 25 cm and 100 cm over two months. It finally went below 2 m at the end of April. Despite this prolonged waterlogged period, observed biomass during the 2014–2015 season was of similar magnitude as other seasons, suggesting that the crop largely recovered once drainage conditions improved. In terms of modelling, the outcome can be different. As discussed in Chapter 3, simulated soil water dynamics under such conditions are highly sensitive to $K_{\text{sat},aq}$, Z_{aq} and, to a lesser extent, $K_{\text{sat},4}$ and the anisotropy ratio. Depending on the value of $K_{\text{sat},aq}$, ponding water can be infiltrated or evaporated by February or persist until early May. This can induce major consequences on crop growth and flux dynamics, because in Daisy, when soil pressure potential reaches zero or above (i.e., saturated or ponding conditions), root water extraction from saturated layers is set to zero. Consequently, there is no nitrogen uptake nor is

there any crop transpiration if the whole profile is saturated.

To constrain these parameters, a measurement campaign was conducted at BE-Lon, in which 29 undisturbed soil cores were collected at five locations within the EC footprint, spanning depths from 7.5 to 100 cm. Each core was equipped with two tensiometers and subjected to the evaporation method (Schindler et al., 2010; Peters et al., 2015), which yields simultaneous estimates of the water retention curve $\theta(pF)$ and the hydraulic conductivity function $K(pF)$. Both were then fitted to the van Genuchten–Mualem model using the LABROS SoilView-Analysis software. The campaign revealed substantial spatial variability. At identical pF in the 80–100 cm layer, measured volumetric water content ranged between 33 and 44% and hydraulic conductivity between 0.01 and 0.16 cm d⁻¹. Fitting the conductivity function was further complicated by the sensitivity of K_{sat} to the Mualem tortuosity parameter L : fixing L at its default value of 0.5 versus fitting it freely caused K_{sat} to differ by a factor of two to four. We finally chose to estimate both, with K_{sat} ranging from 0.0216 to 0.00946 cm h⁻¹ depending on soil depth (Table 3.7).

As the aquitard layer is too deep to directly measure its thickness and saturated conductivity, both aquitard parameters were included in the calibration procedure (Table 4.2). In the most balanced parameter set, the calibrated value of $K_{\text{sat,aq}}$ (i.e., 0.0367 cm h⁻¹) is notably high compared to the conductivities of the overlying soil layers, which seems contradictory with the role of the aquitard layer as a water-blocking layer (Styczen et al., 2004). This raises a concern about identifiability: the calibration targets (NEE, DM and LE) constrain water dynamics only indirectly, through the atmospheric fluxes at the surface. With no direct measurement of soil water flow, the aquitard parameters are effectively tuned against a single season (2014–2015), as shown by their influence (Chapter 3), using variables that are weakly sensitive to subsoil drainage. The calibrated values should therefore be interpreted with caution, as they represent a plausible solution for the calibration objectives rather than a physically verified characterisation of the aquitard.

A key missing constraint throughout this analysis is the absence of direct drain flow measurements at BE-Lon. Two approaches have been used at experimental fields where Daisy has been regularly applied: pressure transducers installed in the drainage outlet (Lindhardt et al., 2001) and automated electromagnetic flowmeters with sub-hourly resolution (Motarjemi et al., 2023). Both give continuous records of discharge that integrate the hydraulic response of the entire soil profile, and are therefore sensitive to both the saturated hydraulic conductivities of the different layers and the aquitard parameters. Drain flow would thus serve as an independent validation variable directly linked to model parameters that cannot be constrained by EC measurements alone (capturing only the atmospheric exchange) or by soil moisture sensors (point measurements that carry no information on lateral drainage). The absence of drain flow data can be seen as a limitation in the calibration carried out in Chapter 4.

Its inclusion in future model evaluation would substantially reduce the uncertainty in hydraulic conductivities parameter estimates, while improving the prediction of water availability and nitrogen cycling during waterlogged periods. On another note, if drain flow is monitored, drainage water could also be sampled for chemical concentrations, enabling the estimation of nitrogen (or even pesticide) leaching (Motarjemi et al., 2023; Holbak et al., 2022; Nagy, 2020).

Besides modelling the water dynamics resulting in waterlogging conditions, Daisy also simulates the plant response to this abiotic stress, which deserves scrutiny at sites as prone to water table rises as BE-Lon. As previously stated, the current implementation sets root water extraction to zero under saturated conditions, which is physically coherent with the closure of aquaporins under anoxia and the consequent reduction of root hydraulic conductivity (Tournaire-Roux et al., 2003; Bramley and Tyerman, 2010). Growth inhibition in the model then follows indirectly from the suppression of nitrogen uptake and transpiration, which propagate to reduce photosynthesis and biomass accumulation. As a comparison, crop models usually represent waterlogged stress through an excess-water or aeration-stress factor applied as a multiplier on one or several growth processes (Githui et al., 2022). AquaCrop and WOFOST apply the stress factor directly to transpiration, the factor in DSSAT influences root growth, water uptake and N-fixation, while APSIM propagates it more mechanistically to root growth, leaf area, photosynthesis and biomass, with a gradual effect depending on saturation duration (Githui et al., 2022; Liu et al., 2020b). Daisy's representation is comparatively coarse: rather than a progressive response, root uptake is switched off entirely once soil pressure potential reaches zero, with no intermediate hypoxic response. This behaviour likely explains part of the sensitivity to $K_{sat,aq}$ and Z_{aq} discussed above, since small changes in simulated ponding duration can shift the crop between fully functional and fully inhibited states, whereas models with gradual aeration-stress functions would dampen this transition.

On the other hand, waterlogging also triggers a suite of additional plant responses that are not represented in crop models (including Daisy): a shift to anaerobic respiration with accumulation of toxic metabolites, morphological adaptations such as aerenchyma development and adventitious rooting, and the re-aeration stress that can follow drainage (Mudasir and Shahzad, 2025; Zhang et al., 2025; Bramley and Tyerman, 2010). Whether these omissions result in meaningful errors at BE-Lon is not fully established. The 2014–2015 season was simulated with reasonable accuracy for biomass (Figure 4.2), but the waterlogged period was not specifically analysed. Identifying and quantifying potential discrepancies during waterlogging events would clarify whether Daisy's simplified representation is adequate for this site or whether the above-mentioned processes and formalisms need to be explicitly implemented.

1.2.2. Edaphic drought stress

Among the studied growing seasons, the driest was 2021-2022. Between 10 April and 20 May, less than 1 mm fell, which led to a measured soil water content reaching 11% at 5 cm depth and 20% at 25 cm depth. It reached, or got close to, the soil wilting point ($pF=4.2$) which was previously measured around 11-14% depending on soil depth, suggesting that access to water can be limited. Moreover, this episode coincides with the period of active vegetative growth and canopy development of winter wheat, when water demand is increasing. Whether this event translated into crop stress, however, is less straightforward.

Root profiles observed at BE-Lon indicated that roots were already present at depths greater than 45 cm by late February and that, at the end of April, 10% of root biomass was found below 60 cm (Hoang, 2022). It means the crop had access to soil layers where water content was less depleted. It is therefore plausible that the crop partially compensated for the dry topsoil by increasing water extraction from deeper horizons, a compensatory mechanism well documented in winter wheat (Bacher et al., 2023; Liu et al., 2023a; Lv et al., 2010). This is also the case in Daisy, where the presence of deep roots in wetter soil layers can partially offset the deficit in drier upper layers. During this episode, simulated water uptake in the upper soil layer (0–15 cm) stopped around 13 May and, more specifically, no water uptake from 0–5 cm occurred after 28 April. Most of the water was obtained from the 20–45 cm soil layers. It is, however, worth noting that simulated rooting depth was around 15 cm on 15 April and 40 cm on 20 May, which are much shallower than observed. If the dry episode occurred earlier in the season, simulation outputs would greatly vary from observations as roots would not be deep enough to reach layers with higher water content. Furthermore, parameters describing root penetration were considered as species-specific, rather than cultivar-specific (Acuña and Wade, 2013; Nakhforoosh et al., 2014), which also contributes to the misrepresentation of the root profiles. All things considered, this is thus a serious limitation of the current parameterisation that needs to be addressed in future work.

In Daisy, under edaphic drought, transpiration and carbon assimilation are reduced due to stomatal closure. The sensitivity of stomatal conductance to soil water availability is partly governed by the parameter δ (Equation (2.11)), which was adjusted in Chapter 4. Among the four seasons considered, the highest calibrated value of δ was obtained for 2021–2022 (Table 4.4), consistent with the dry conditions observed and suggesting that it required a stronger stomatal limitation to reproduce the measured fluxes. Compared to other widely used models, drought representation in Daisy, which depends on crown potential and ABA, is more sophisticated (Verhoef and Egea, 2014). To down-regulate processes, crop models and LSM usually use an empirical water availability factor β which, for instance, corresponds to the relative extractable water (REW) in WOFOST, APSIM, JULES and CTESSSEL (Dhakar et al., 2018; Best et al., 2011; Boussetta et al., 2013). Easy to implement, these empirical factors are

increasingly criticised for their unrealistic drought responses due to abrupt transitions (Powell et al., 2013). This criticism does not apply to Daisy, as the stomatal reduction is a continuous function of crown water potential (Equation (2.11)), rather than a threshold. However, in order to assess the complete drought representation in Daisy, ABA observations are required, which is a major constraint. As previously explained, only the hydraulic signalling (i.e., dependence on crown water potential with δ) was considered in this thesis, as ABA data were not available. Future work with dedicated measurements should evaluate the contribution of chemical signalling for improving drought response and compare it with promising alternatives such as the incorporation of plant hydraulics theory (Kennedy et al., 2019; Alléon et al., 2025).

Besides the water availability factor itself, there is a wide variability in which processes are impacted. In LSM, this factor is usually applied to the stomatal conductance (Zhou et al., 2019). In addition, CLM (version 4.5 and before) also applies it to $V_{c,max}$ and dark respiration (Oleson et al., 2013). More recently, a β factor was also applied to the mesophyll conductance when incorporated into JSBACH and JULES (Knauer et al., 2020; Vidale et al., 2021). In crop models, transpiration and carbon assimilation are usually impacted by the water availability factor, but it can also influence crop development. Phenology (emergence, flowering) can be delayed under soil water stress in APSIM, STICS and DSSAT. Leaf expansion can be influenced by modifying the specific leaf area in STICS and DSSAT. Similarly, leaf senescence is accelerated under water deficit in STICS and WOFOST. And, finally, dry matter partitioning can also be impacted by water stress in DSSAT, with a shift towards roots (Dhakar et al., 2018). In comparison, Daisy routes all drought stress through the stomatal pathway, with emergence delay as the only additional process. The supplementary effects on leaf expansion, senescence, mesophyll conductance and carbon allocation that other models represent are absent, which may lead to an underestimation of drought impacts on final yield in seasons where stress is sustained and severe enough to trigger these secondary responses.

To fully assess Daisy's drought representation and which additional processes should be impacted, the 2021–2022 season is insufficient. The compensatory uptake from deep roots likely buffered the crop from severe water stress. This is moreover coherent with the cross-model comparison between FvCB and MLR. During this season, the MLR model predicted higher photosynthesis than FvCB (Figure 5.2). Because the MLR model is driven by the SIF signal, and SIF reflects the actual photosynthetic electron transport activity, a severely stressed crop would exhibit increased NPQ and reduced PSII efficiency, both of which would suppress the SIF signal and lead to lower GPP rather than higher. This is further supported by Beauclaire et al. (2024a), where REW was found not to affect leaf-level quantum yields, confirming that photochemical efficiency was not impaired during the dry episode. A more diagnostic evaluation of Daisy's drought representation would require a season in which severe drought is established without deep water access. Without such a contrasting case, the question

of whether Daisy stomatal-only regulation is adequate for drought-limited conditions for winter wheat remains open.

1.2.3. Heat stress

As shown in Chapter 4, a 5-day period with high temperature and VPD was reported during the 2018–2019 growing season. Although not discussed in that chapter and often shorter, similar events occurred in all studied seasons. For each of these events, observations followed the same trend: LE significantly increased, but NEE (and estimated GPP) did not. This decoupling between transpiration and carbon assimilation needs to be reproduced by the model and is deeply discussed hereafter.

But before diving into this decoupling, a first question is how well Daisy resolves the thermal environment experienced by the canopy. Many crop models operate on daily timesteps and apply temperature functions to mean daily temperature, blurring the distinction between moderate and extreme conditions occurring within the same day (Richetti et al., 2025). Operating at an hourly resolution, Daisy estimates leaf temperature separately for sunlit and shaded fractions of the canopy, accounting for the radiative and turbulent energy balance of each component (Plauborg et al., 2010). This places Daisy closer to LSM than to most crop models in terms of thermal representation, enabling a better estimation of the thermal magnitude experienced by the canopy.

Temperature influences most of the photosynthetic processes in Daisy explicitly. Carboxylation capacity ($V_{c,max}$) and electron transport rate (J_{max}) both follow temperature response functions with an optimum and a high-temperature decline, and dark respiration increases exponentially with temperature. At optimum temperatures (30–35°C), higher assimilation tends to increase g_s through the Leuning model, which in turn promotes transpiration. However, the relationship between temperature and stomatal aperture is not as straightforward because of the thermodynamic coupling between air temperature and VPD: saturation vapour pressure increases nonlinearly with temperature, so moderate warming produces a rapidly increasing VPD at constant relative humidity (Grossiord et al., 2020). In the Ball-Berry family of models, including Leuning, VPD enters as a direct down-regulator of g_s . Therefore, temperature and VPD act as antagonistic drivers on stomatal aperture, and their effects can partially compensate.

Recent studies have managed to isolate the temperature effect from VPD in order to analyse the carbon–water relationship with temperature independently (Diao et al., 2024; Urban et al., 2017b). Compared to the logic outlined above, where changes in carbon assimilation and transpiration track each other through their shared dependence on g_s , Diao et al. (2024) observed the opposite at high temperature. Photosynthesis declined while transpiration and g_s continued to increase. Furthermore, they also found g_m to decline above approximately 20–25°C, while the CO₂ concentration at the carboxylation sites C_c remained relatively constant. This means that the reduction in net assimilation under high temperature cannot be attributed to reduced CO₂ supply

through the stomata (as they were open) but reflects instead a biochemical limitation at or downstream of the mesophyll, operating independently of stomatal aperture. This decoupling between transpiration and carbon assimilation is precisely the pattern observed at BE-Lon during heat episodes: LE increases while NEE declines or stagnates.

Several mechanisms have been proposed to explain it, including thermal inactivation of Rubisco and decline in electron transport rate, while stomata remain responsive to other signals (Urban et al., 2017b; Salvucci and Crafts-Brandner, 2004). What these mechanisms share is that they operate independently of the $A-g_s$ coupling assumed in Ball-Berry models. In other words, the carbon and water pathways diverge. FvCB-based models coupled to Ball-Berry stomatal conductance, including Daisy, cannot simulate this divergence. The model systematically underestimates transpiration under heat stress by assuming a tighter carbon–water coupling than observed. Furthermore, using the MLR model showed no systematic improvement over FvCB in reproducing NEE and LE during those specific days, although any downregulation of PSII activity would be captured by the SIF signal. The absence of improvement suggests that the failure is not located in the photosynthesis module itself but is structural and shared by both models. It lies in the stomatal conductance model, which controls transpiration, and in the missing non-stomatal pathways that allow the two fluxes to decouple. Reproducing this divergence in a model requires, at minimum, an explicit temperature response of g_m . Ideally, the thermal sensitivity of Rubisco activity and electron transport should not be tied to the stomatal conductance, and the temperature effect on g_s should be further analysed, as previous studies have provided conflicting results (Urban et al., 2017b).

Given how central measured NEE and LE are to this situation, it is also worth discussing their potential biases. When measuring turbulent fluxes, one major source of bias is the correction of spectral attenuation of the signal. In a recent multi-site comparison of spectral correction approaches, Faurès et al. (2026) highlighted weaknesses in the ICOS procedure. Comparing their method to ICOS, they found an average difference of 1.6% and 10.7% for, respectively, CO₂ and H₂O cumulated fluxes, with BE-Lon having the biggest difference for H₂O. For this entire work, flux data were corrected following their recommendations. Another potential bias has been briefly discussed in Section 4.2. Eddy covariance systems generally underestimate turbulent energy fluxes, which is known as the surface energy balance closure problem (Nicolini et al., 2026; Mauder et al., 2020). Because Daisy explicitly resolves the surface energy balance rather than estimating LE independently, comparing it against non-closed observations would introduce a bias unrelated to any process represented by the model. Even for a perfectly performing model, non-corrected LE would appear systematically lower than simulated LE. The corrected fluxes (LE_CORR and H_CORR), obtained from the standard closure procedure implemented in the ONEFlux pipeline (Pastorello et al., 2020), were therefore used throughout this thesis. However, this choice is not free of uncertainty. The closure correction assumes that the residual energy can be

attributed to H and LE depending on the Bowen ratio, an assumption that remains actively discussed in the eddy covariance community and is currently being re-examined for BE-Lon within the AGROFLUX project. On the other hand, no correction was applied for NEE. While it is suggested that CO₂ fluxes are also underestimated (Gao et al., 2019; Mauder et al., 2024), using the same reasoning as for energy fluxes (i.e., due to sub-mesoscale organised structures), there is currently no recommended correction method for NEE (Section 4.2).

1.3. Is such a workflow always recommended?

The workflow adopted in this thesis, i.e. temporal GSA followed by multi-objective calibration and validation, was demanding. It required running Daisy tens of thousands of times, developing temporal sensitivity diagnostics and interpreting Pareto fronts rather than a single optimum. This raises a legitimate question: was this level of methodological investment necessary and would it be equally justified for other modelling exercises?

Several elements of this thesis suggest that the answer depends on how mature the model configuration already is. The SVAT component of Daisy, coupling FvCB photosynthesis and Leuning stomatal conductance to the surface energy budget, is comparatively new and has not undergone the same iterative refinement as the soil-focused core of the model. In this context, GSA was not simply a preliminary step before calibration but also provided useful insights. In addition to quantifying the influence of Daisy parameters for the first time in an integrated way, the temporal GSA revealed errors that would have gone unnoticed otherwise (Chapter 3). Similarly, early attempts to calibrate Daisy with more standard approaches, including a Bayesian calibration against weighted objectives following Minet et al. (2015), failed to converge to a stable posterior parameter distribution. It is only once the Pareto-based multi-objective calibration had exposed the conflicting nature of the objectives, that this earlier lack of convergence could be understood. The Bayesian method was implicitly attempting to average away trade-offs that the model cannot resolve itself, given its current structure and data used. This illustrates a broader point: when a model exhibits genuine multi-objective trade-offs, single-objective and weighted-sum approaches can fail silently, either converging to a compromise solution with no clear physical meaning or failing to converge at all, without indicating why. Pareto-based multi-objective methods make such conflicts explicit rather than hiding them in a scalar loss function, which is precisely what allowed the diagnostic interpretation carried out in Chapter 4.

This diagnostic value, however, comes at a cost that may not always be justified. For study applications using a well-established model configuration that have been assessed with similar data and conditions, most of the structural issues that this workflow revealed have typically already been identified and addressed in earlier studies. In such cases, a lighter sensitivity and calibration procedure is likely sufficient. Although

two-step GSA (screening followed by a variance-based method) is increasingly recommended (Wang et al., 2025; Gilardelli et al., 2018), time-efficient alternatives are also worth exploring and comparing. For instance, in the AgMIP protocol, the selection of parameters to calibrate is based on the corrected Akaike information criterion, which is designed to avoid over-parameterisation (Wallach et al., 2025; Wallach et al., 2024). Likewise, if no significant trade-off exists between calibration objectives, other multi-objective techniques can be used which require less analysis effort than an explicit Pareto search. These include the frequentist approach GLUE (Mo and Beven, 2004), which embraces equifinality but does not resolve trade-offs explicitly, the Bayesian approach DREAM and its derived versions (Vrugt et al., 2008; Minet et al., 2015) or even the weighted least squares (Seidel et al., 2018; Wallach et al., 2025) where objectives are aggregated into a single one.

All things considered, we suggest that a full temporal GSA and Pareto-based multi-objective calibration workflow is recommended, particularly when (i) the model configuration under study is relatively novel, less tested, or being applied at a new site or under new conditions, and (ii) multiple, physically distinct observations are available that could constrain the simulated processes differently. In this sense, this workflow should not be regarded as a default calibration procedure to be applied uniformly, but rather as a diagnostic tool of choice for the early or exploratory stages of model application, whose cost is best justified by the depth of structural insights it can provide.

1.4. Concluding remarks

In conclusion, Daisy is a suitable tool for modelling cropland flux dynamics while enabling the simulation of wide range of human-managed actions (e.g., ploughing, stubble breaking, organic and mineral fertilisation) and crop development processes (e.g., phenology stages, leaf and root senescence, reserve remobilisation, incorporation of crop residues). The overarching question of this thesis was addressed through five research questions, whose main answers are summarised in Figure 6.1. Throughout this thesis, the consecutive chapters demonstrate both the potential and the current limits of Daisy. Despite the trade-off identified, net ecosystem exchange and dry matter can be simulated with reasonable accuracy. However, latent heat flux is less reliable and deserves further improvement. We also pinpoint what is needed to better assess Daisy's response to abiotic stress, namely non-stomatal limitations for the response to heat, drain flow data for waterlogging episodes and an evident drought season to challenge the drought response.

The development priorities of the Daisy team naturally reflect their core expertise in soil dynamics, as illustrated by the recent advances in the simulation of fractures and large biopores with specific transport equations for water and solute (Holbak et al., 2021) or the consideration of dissolved organic matter (Gjettermann et al., 2008). Atmospheric exchanges are integrated and maintained, but improving the SVAT and FvCB–Leuning coupling, to address the issues raised in this work, would require sustained effort from users working at the interface of soil-plant-atmosphere modelling, rather than from the core team. The open-source nature of Daisy makes such contributions genuinely feasible, as the corrections and amendments carried out during this thesis were straightforward to implement and to share with the development team.

Addressing these issues, particularly the trade-off between DM and NEE, is crucial for GHG mitigation policies. As policy frameworks, such as the 4 per 1000 initiative, aim to promote, reward or certify carbon storage in agricultural soils, they rely on credible estimates of how soil carbon evolves under different practices and climatic conditions. However, this DM–NEE trade-off points to an imbalance in the carbon budget of the model or to biases in the EC measurements, which limits the assurance that can be placed in such model estimates and measurements. Once it is resolved, Daisy could be confidently used for simulating the evolution of soil carbon over crop rotations. Repeated soil inventories only capture this evolution over long intervals and with large uncertainties, so a process-based model constrained by flux and biomass observations could complement them. On a different note, and despite the focus on carbon and water in this work, it should be recalled that Daisy also simulates soil nitrogen processes. While N_2O fluxes were only considered in Chapter 3, they were later discarded because of the lack of data and model quantification for denitrification. As a result, Daisy prediction of N_2O fluxes were not calibrated nor assessed for BE-Lon, although it is valuable for GHG mitigation.

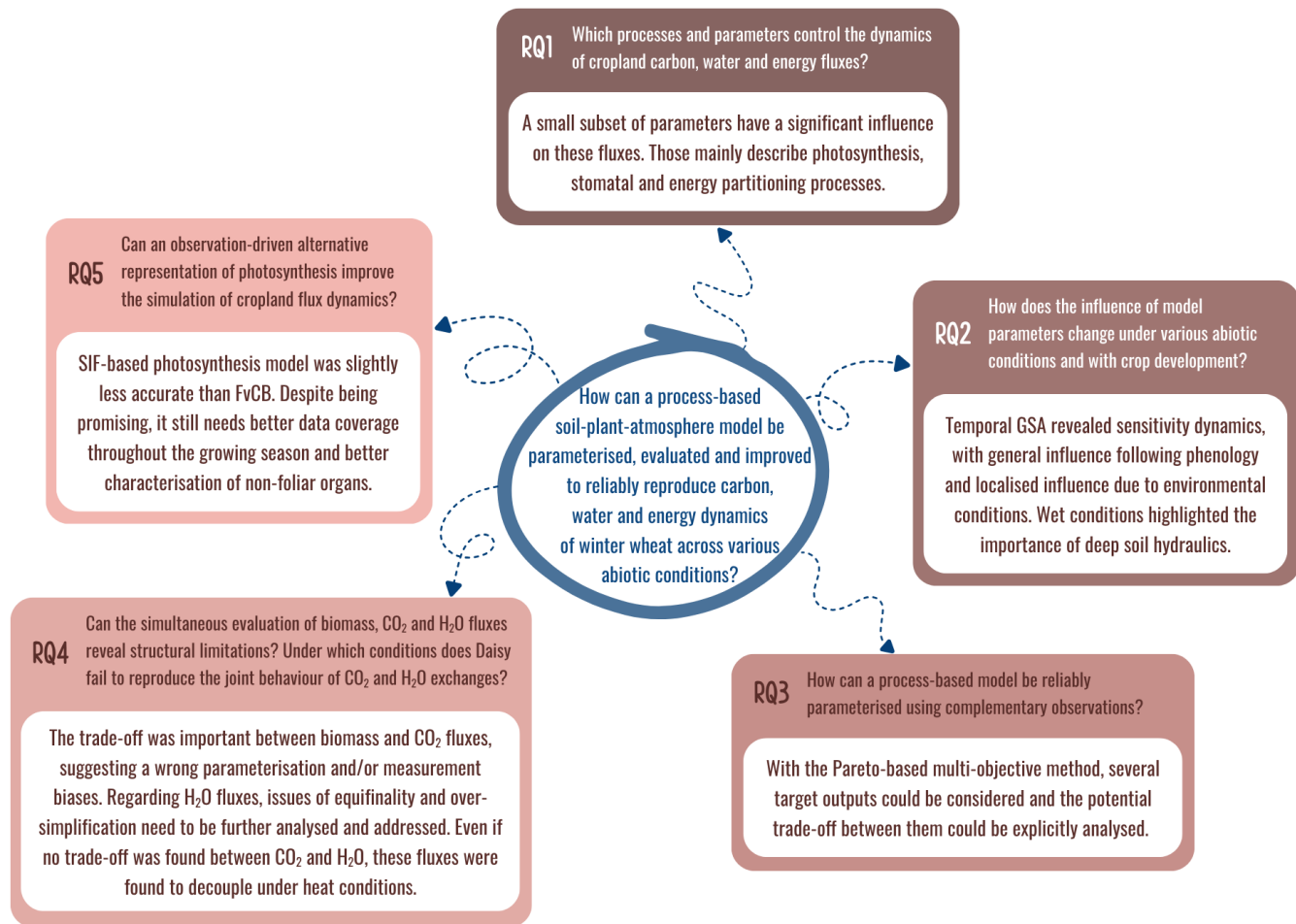


Figure 6.1: Thesis summary and take home messages.

2. Going a step further

2.1. *Resolving NEE-DM trade-off*

The persistent trade-off between NEE and DM identified in Chapter 4 points to an imbalance in the carbon budget of the model. As this trade-off was often accompanied by an underestimation of crop yield (i.e., DM in storage organs), we first integrated the photosynthesis of non-foliar organs in order to increase the synthesised assimilates during the grain filling period and mitigate the trade-off. Even though the photosynthetic efficiencies of these organs (stem and storage organs) were added as targeted parameters in Chapter 4, the trade-off was still present. We then tried to adjust the partitioning coefficients, reduce the maintenance respiration after anthesis, which could further be expressed as a function of tissue N content (Delandmeter et al., 2023), and modify the parameters related to the heterotrophic respiration (Section 6.1), but neither alleviated the trade-off.

Instead of blindly testing solutions, we need additional measurements. As stated above, EC systems do not distinguish between NEE components. However, measuring photosynthesis, autotrophic and heterotrophic respiration separately would allow to confirm or rule out some of the explanations reported in Chapter 4. Such measurements would require a dedicated campaign and experimental design. Soil respiration can be directly measured using soil chambers, but the measured CO₂ efflux consists of heterotrophic respiration as well as root autotrophic respiration that need to be separated. Many separation techniques exist, ranging from isotopic methods (Hagedorn et al., 2010) to difference methods such as root exclusion (Sun et al., 2019; Suleau et al., 2011), trenching (Hu et al., 2018; Savage et al., 2013) or tree girdling (Högberg et al., 2001), as defined by Kuzyakov and Larionova (2005). At BE-Lon, Suleau et al. (2011) prepared root exclusion zones of 3 × 3 m for estimating each respiration component. By doing so, rhizomicrobial respiration (as defined in Section 1.2) was wrongly merged with autotrophic root respiration, leading to a possible underestimation of heterotrophic respiration. Similarly, each method has its own shortcomings, hence they are often combined to better characterise soil respiration (Comeau et al., 2018; Kuzyakov and Larionova, 2005).

Despite the drawbacks of the method used by Suleau et al. (2011), this is still a first attempt to estimate respiration components at BE-Lon. The resulting fitted function helped us identify the possible underestimation of heterotrophic respiration by Daisy, but this is not entirely transposable. It would have been interesting to simulate the winter wheat season of 2006-2007, which was studied by Suleau et al. (2011). During this

season, regular measurements of vegetation area index and biomass (with distinction for stem and ear) were conducted over a longer period than usual, as first measurements were reported before January. Unfortunately, this season was discarded at the beginning of this thesis because of the lack of information on dead leaves as well as on water table depth, the low data coverage for sensible heat fluxes and the EC set-up being overall less equipped before 2014.

In addition to simulating the 2006-2007 season, a new measurement campaign could give other useful insights and address the limitations present in Suleau et al. (2011). By combining isotopic and difference methods, the relative contributions of microbial, root autotrophic and rhizomicrobial respiration could be disentangled more rigorously (Song et al., 2016; Carbone et al., 2016). Such a campaign should also include measurements specifically targeting the grain filling period, which was identified as critical and poorly reproduced in both Chapters 4 and 5. In particular, gas exchange measurements on non-foliar organs (i.e., ears, glumes and flag leaf sheaths) would help quantify their contribution to carbon assimilation, which the model currently represents through fixed photosynthetic efficiency parameters that showed large variability between seasons. Finally, regular measurements of stem water-soluble carbohydrates throughout the reproductive stage would allow the dynamics of remobilisation to be directly quantified and compared against model predictions. This would help establish whether the underestimation of grain yield is primarily a remobilisation, an allocation or a photosynthesis problem. Together, these measurements would transform the current situation into a better-constrained problem that could result in model improvement.

As reported in Chapter 4, the last explanation worth exploring is the systematic bias in NEE measurements. Nearly 20 years ago, the non-closure of ecosystem carbon budgets was already reported for EC sites (Luyssaert et al., 2007). They introduced correction terms to close the CO₂ balances that substantially accounted for 10 to 60% of GPP. This CO₂ non-closure is supported by a recent study comparing soil inventories, simulation of soil organic carbon (SOC) by RothC and EC-based carbon budget at BE-Lon (Beauclaire et al., 2026). Whereas soil inventories and process-based modelling suggested that SOC reached a quasi-equilibrium (respectively, a loss of $6.33 \pm 11.23 \text{ gC m}^{-2} \text{ y}^{-1}$ and a gain of $19.7 \pm 30.3 \text{ gC m}^{-2} \text{ y}^{-1}$), a significant loss of $69.8 \pm 19.2 \text{ gC m}^{-2} \text{ y}^{-1}$ was reported using EC data. Assuming that the CO₂ balance is not closed and lateral fluxes are correctly estimated, they found that EC measurements captured only 82.7% of the true CO₂ exchange over the cropland. If the above-mentioned measurements are implemented at BE-Lon, along with the next soil inventory scheduled for 2027, it could help us identify if EC measurement biases are the source of this trade-off or which part of Daisy is responsible.

2.2. *Integration of non-stomatal limitations*

A particularly striking result from Chapter 4 was the model's failure to reproduce the stomatal behaviour of winter wheat during a heatwave episode in April 2019. As further explained in Section 1.2.3, measured LE continued to increase, suggesting that the crop increased transpiration, while sustaining its photosynthesis rate. It revealed a decoupling between carbon and water fluxes that the FvCB-stomatal conductance coupling in Daisy could not reproduce. This observation is consistent with the concept of non-stomatal limitations to photosynthesis under heat stress (Flexas, 2002). It includes restriction of CO₂ diffusion through the mesophyll or biochemical alteration of photosynthetic apparatus (Beauclaire et al., 2023).

Although its role in limiting photosynthesis has been recognised for decades (Flexas et al., 2012), g_m is rarely incorporated in crop or land surface models due to the difficulty of its measurement and parameterisation (Vidale et al., 2021). Some recent examples include its integration in JSBACH (Knauer et al., 2019), in JULES (Vidale et al., 2021), in SIBCASA (Van Der Velde et al., 2018) and in ORCHIDEE (Abadie et al., 2025). Its formalism varies widely among these models, with a g_m depending on $V_{c,max}$ of top sunlit leaves, photosynthetic rate and soil water stress for SIBCASA, whereas, in JSBACH, the reference g_m (25°C) is multiplied by the effects of leaf nitrogen content, leaf temperature, soil moisture content, C_i and absorbed PPFD.

The S22 dataset collected at BE-Lon offers a great opportunity to quantify g_m as well as its response to environmental drivers. It comprises leaf-level gas exchange measurements and chlorophyll fluorescence data, which together allow g_m to be estimated using the variable J method (Harley et al., 1992), as described by Beauclaire et al. (2024b). Hence, an empirical or semi-mechanistic g_m parameterisation, similar to those mentioned above, could be integrated into a modelling framework like Daisy. Furthermore, such implementation could be tested on the potato growing season of 2020, during which similar data were acquired and g_m was reportedly the key limitation on carbon fluxes (Beauclaire et al., 2024b).

2.3. Beyond winter wheat

The modelling workflow and developments made in this thesis were applied specifically to winter wheat at BE-Lon. An important question for the broader applicability of the results is how transferable it is to other crops and environments. The BE-Lon rotation includes sugar beet, potato, seed potato and winter wheat in succession, for which biomass and flux data are available. In her master's thesis, Radelet (2025) aimed to reproduce the 2016-2020 crop rotation with a focus on the impact of soil labour and cover crops on GHG fluxes. Afterward, Lemaire (2026) continued to work on the same rotation, but his thesis was more centred on the bioincorporation of crop residues. These theses show that Daisy can be applied to crops other than wheat with relatively good results, although neither a thorough sensitivity analysis nor calibration was conducted for this entire rotation. Extending the calibration to the full rotation would test whether the soil parameter set identified for winter wheat remains valid when a different crop occupies the field, or whether recalibration is necessary, as well as verify if the trade-off between NEE and DM is specific to winter wheat or if it exists for other crops as well. More fundamentally, simulating the full rotation would enable Daisy to be used for long-term gap-filling and carbon balance estimation across a multi-year period, which could help reconcile the unexpectedly large carbon deficit identified in the long-term EC record at BE-Lon (Buysse et al., 2017).

2.4. Extending to other sites

Daisy, as well as the modelling workflow developed in this thesis, can also be applied beyond BE-Lon. Doing so would address a question that this thesis cannot answer on its own: which of the findings are specific to this site and which reflect more global properties of the Daisy model or of temperate croplands more broadly.

Two complementary options are worth distinguishing. The first is the ICOS cropland network, which currently includes several European sites covering a range of climates, soils and management systems. Standardised measurement protocols and data quality flags across ICOS sites mean that the same calibration and validation procedure applied here could be reproduced with minimal preprocessing effort, enabling a direct comparison of dominant sensitive parameters and calibrated parameter values across sites. Such a comparison would reveal, for instance, whether the DM-NEE trade-off identified in Chapter 4 is a structural limitation of Daisy that emerges across all cropland sites or whether it is specific to the soil carbon dynamics and heterotrophic respiration rates at BE-Lon.

The limitation of ICOS sites, however, is that they are monitoring platforms: management and land use are fixed and cannot be adapted to target specific model limitations. Applying Daisy at dedicated experimental fields would remove this constraint. At such sites, it would be possible to design an experimental study in direct response to the uncertainties identified here: for example, installing multiple soil chambers for

respiration partitioning, with larger and more easily maintained root exclusion zones. Or clearly identify the impact of soil water stress by conducting controlled treatments. Existing experimental fields with similar pedoclimatic conditions as BE-Lon would provide a natural starting point, such as the experimental parcels in Bordia (Gembloux), managed by Gembloux Agro-Bio Tech (Lognoul et al., 2017) or the Longs Tours site also located in Gembloux and managed by the Walloon agricultural research centre (Buysse et al., 2013).

Altogether, these two options are not mutually exclusive. ICOS sites offer a fast route to cross-site comparison, while dedicated experiments offer the targeted data needed to resolve specific process uncertainties. Pursued jointly, they would move this evaluation of Daisy from single-site case studies towards a more robust, generalisable understanding of temperate cropland carbon and water dynamics.

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