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Water and carbon fluxes in young plantations: observations and modelling

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Abstract

The establishment and expansion of commercial plantations for timber production and carbon sequestration raise concerns because of their large water use. The dearth of high resolution experimental observations and knowledge of the dynamics of water use and growth in plantations, especially in their early years after establishment, makes it difficult to develop better management practices. Investigating ecosystem responses to environmental variables can provide insights on how plantation trees adjust their water use according to local conditions.

Combining field measurements and hydrodynamic modelling, this project provides a unique and comprehensive quantification of the trade-offs between water use and carbon assimilation in a *Eucalyptus globulus* (blue gum) plantation in the first 4 years after establishment. The blue gum is one of the most planted species globally, as it grows rapidly and is adaptable to a range of climatic conditions. The experimental measurements were performed in a study site located in southwest Victoria, Australia, where energy and CO₂ fluxes were continuously measured above the tree canopy for 3.5 years after the trees were planted. During the first year after establishment, understory vegetation and ecosystem respiration had a major impact on the net ecosystem exchange (NEE), with the plantation being a net carbon source. Subsequently, the trees started dominating the contributions to NEE and, after approximately 2 years, the plantation became a consistent carbon sink. These shifts in NEE were accompanied by smaller increases in annual evapotranspiration rates, which was 70% of the annual precipitation in the first year and 74% in the third year of measurements. This shows a remarkable increase in productivity at the expense of a small amount of water.

To further understand and estimate transpiration dynamics in plantation trees, a tree hydrodynamic model (FETCH3) was developed. FETCH3 assumes that the water flow through the soil, roots, and above-ground xylem can be approximated as flow in porous media. Through the application of the Richardson-Richards equation, FETCH3 describes the transport of water through the plant system by applying a rigorous coupling of the soil, roots xylem, and stem xylem pathways. The numerical scheme of the model, developed in Python 3, was verified and produced considerably small errors against exact analytical solutions for steady state and transient conditions using simplified but realistic model parametrizations. The model was also used to simulate a previously published case study where observed transpiration rates were available and the results were in agreement with observations. Finally, the model was calibrated using transpiration data collected from sap flow sensors installed in growing blue gum trees in the study site.

The results from this project emphasized the highly dynamic water and carbon fluxes in young and recently established plantations trees. Specifically, the continued cultivation of large scale commercial plantations would benefit from management practices that are inclusive of information and data from all the years of the management cycle, including the first few years after establishment.

Declaration

This thesis is an original work of my research and contains no material which has been accepted for the award of any other degree or diploma at any university or equivalent institution and that, to the best of my knowledge and belief, this thesis contains no material previously published or written by another person, except where due reference is made in the text of the thesis.

Signature:

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Date: 27th July 2022

Publications during enrollment

- **Silva, M.**, Matheny, A. M., Pauwels, V. R. N., Triadis, D., Missik, J. E., Bohrer, G., and Daly, E.: Tree hydrodynamic modelling of the soil plant atmosphere continuum using FETCH3, Geosci. Model Dev., 2022. (I.F. 7.708, Q1 in Earth and Planetary Sciences and Model and Simulation)
- **Silva, M.**, McHugh, I., Peixoto Neto, A., Pauwels, V.R.N., Cartwright, I., Daly, E.: Trading a little water for substantial carbon gains during the first years of a Eucalyptus globulus plantation, Agricultural and Forest Meteorology. (I.F. 5.734, Q1 in Agronomy and Crop Science, Atmospheric Science, Forestry, and Global and Planetary Change)

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Chapter 1

Introduction

The area planted with forests has increased world-wide by 123 million hectares since 1990 and covered 294 million hectares in 2020. Approximately 45 percent of the planted forests are plantations, which are intensively managed forests, mainly composed of one or two tree species, native or exotic, of equal age, planted with regular spacing and mainly established for productive purposes (Downham and Gavran, 2020; FAO and UNEP, 2020). Plantations have expanded in order to supply the demand for timber production and as a tool for carbon storage (Benyon et al., 2009; Landsberg and Waring, 1997). Despite their economic importance, large-scale plantations have been criticised because of the higher transpiration and interception rates associated with trees, resulting in a greater water use and soil nutrient depletion (David et al., 1997; Jackson, 2005; Tfwala et al., 2019). Especially in semi-arid regions, limited precipitation calls for regulations of water allocated to commercial plantation activity, creating tensions between land owners, plantation companies, and water planners (Greenwood, 2013; White et al., 2016).

In Australia, where commercial plantations cover approximately 2 million hectares, fast-growing species, such as the *Eucalyptus globulus* (blue gum), are planted for hardwood production (Downham and Gavran, 2020). Blue gums are one of the world's most planted and economically important hardwood species (Tomé et al., 2021). The environmental impact of afforestation with fast-growing species is not clear yet due to limited studies measuring tree water use during the entire management cycle (Benyon et al., 2006; Cabral et al., 2011; Cleverly et al., 2020; Forrester et al., 2006; Hinko-Najera et al., 2017). There are even fewer studies dedicated to provide knowledge regarding growth, water use and water use efficiency of young plantation stands (Dye and Versfeld, 2007; Dye, 2000).

In this context, knowledge on plantation water and carbon fluxes can assist in determining the dynamics of plantation carbon gains against the amount of water used by trees (White et al., 2021). As such, there is a need for a better understating of tree water use, in particular intra-daily and intra-seasonal temporal scales, in order to understand and quantify how trees respond

to differences in environmental conditions (Cleverly et al., 2020; Migliavacca et al., 2021). The estimation of water and carbon trade-offs can be critical for agricultural management decisions and to predict how climate events, such as heatwaves or intense rainfall, can influence the physiology, productivity, and water use of *Eucalyptus* forests (Baldocchi et al., 2018). This information is useful for both plantation companies, which can increase productive rates and profit, and water agencies, which can organize governmental license procedures (Benyon et al., 2009; Greenwood, 2013).

Therefore, this project aims to improve the understanding and provide realistic estimations of plantation water use and carbon assimilation, bringing additional knowledge through experimental measurements and modelling of tree water use dynamics. Specifically, this project focuses on the relationship between afforestation, environmental variables, and water use in young and fast growing plantations, since it is still undetermined and sparse in literature (Chan et al., 2018; Ma et al., 2019).

Chapter 2 of this thesis contains a literature review on the dynamics of plantation water and carbon fluxes. The chapter starts reviewing the impacts of plantation activity on the water balance of rural catchments, followed by the description of the development of the plantation industry in Australia. Next, the literature review discusses the drivers of water and carbon fluxes and the water use efficiency in plantation ecosystems, lastly focusing on young and recently established plantations. A review of modelling approaches to assess plantation water use is also included, with the tree hydrodynamic modelling being highlighted as an alternative to represent intra-daily dynamics of transpiration and to realistic represent plant traits.

Chapter 3 presents the results of measurements of energy and carbon fluxes in a young *Eucalyptus globulus* plantation during its first 4 years after establishment. The fluxes were measured using the eddy covariance method with the equipment raised above the canopy as the trees grew; additional measurements of tree height and diameter at breast height were taken to monitor tree growth. The different dynamics in water and carbon fluxes for young stands captured described in this Chapter highlighted the need to evaluate stand age and species-specific characteristics.

Chapter 4 introduces the The Finite-difference Ecosystem-scale Tree Crown Hydrodynamics (FETCH3), a ready-to-use open-access model that simulates the water fluxes across the soil-plant-atmosphere continuum. The chapter describes the derivation of the governing equations and provides the detailed numerical scheme for the solution of the three coupled partial differential equations defining the water fluxes across the system. The numerical solution includes an improved coupling between the soil, roots, and stem xylem. Lastly, the different formulations for the transpiration, root water uptake, hydraulic conductance, and capacitance functions are presented.

Chapter 5 evaluates FETCH3 against different applications. FETCH3 was tested against ana-

lytical solutions (unsteady and steady state formulations) and against a published case study, when the modeled transpiration was compared to observed sap flux data over a period of 5 months. Lastly, the Chapter describes the calibration process against measured sap flow data through the application of the Particle Swarm Optimization (PSO) algorithm.

Chapter 6 summarizes this thesis. The chapter outlines the results of the study, both in terms of experimental measurements and FETCH3 modelling applications, highlighting the contributions of the research and providing several suggestions for future research efforts.

Chapter 2

Literature Review

2.1 Impact of afforestation on rural catchments

The conversion of land from native or agricultural vegetation to commercial plantations is occurring in several countries, and over extensive areas of the southern hemisphere (Farley et al., 2005; Saadaoui et al., 2017). Since the 1950's, the establishment of commercial plantations has expanded, especially the genus *Eucalyptus*, which is the most common plantation worldwide (Tomé et al., 2021). Plantations areas expanded in several countries, including Brazil (Almeida et al., 2007), India (Calder, 2007), China (Chan et al., 2018; Ma et al., 2018), Chile (Acuña et al., 2018), South Africa (Dye, 2013, 2000), and Australia (Almeida et al., 2010; Downham and Gavran, 2020; Forrester et al., 2010a).

Interest has been growing for high productive tree species, given the potential for pulp and paper industries development (Calder, 2007). Another contributor for plantation expansion is the market incentives to reduce CO₂ atmospheric concentrations through carbon-sequestering projects, which include afforestation and reforestation (Fatichi et al., 2019). Additionally, commercial plantations generate a source of income for rural areas (Dye, 2000). However, expansion of commercial plantations has raised controversy because of the high water use associated with short-rotation plantations, especially in semi-arid areas (Greenwood, 2013).

Land-use change due to afforestation has the potential to affect ecosystem processes, such as transpiration, interception, and evaporation, and possibly alter stream flows and groundwater recharge (Brown et al., 2005, 2015; Dye, 2013; Jackson, 2005). These changes can subsequently alter catchment water budgets, supply, and quality (Dresel et al., 2018). To clarify the magnitude and the links between afforestation and water yield, paired catchment studies are commonly used to investigate the impacts of land-use change due to afforestation or deforestation on the catchment water yield.

Paired catchment studies estimate alterations on stream flow due to increases in evapotran-

spiration and interception rates by the vegetation cover (Brown et al., 2005; Dean et al., 2016; Dye, 2013). They are based on two catchments with similar characteristics, such as slope, soils, climate and vegetation, and commonly a short distance from each other. After a period when both sites are monitored, known as calibration period, one catchment land cover is modified. Hence, this type of analysis is useful to understand how streamflow, as a consequence the water balance, is altered in comparison to different treatments and vegetation cover (Brown et al., 2005).

Several paired catchment studies have examined streamflow or evapotranspiration changes caused by afforestation. However, the relationship between land use and streamflow is still not completely understood, with studies documenting considerable streamflow reduction with afforestation (Adelana et al., 2014; Bonnesoeur et al., 2019; Brown et al., 2005; Vertessy et al., 2001; Zhang et al., 2011, 2012) and, contrarily, other studies not finding any significant changes after plantation establishment (Brown et al., 2015; Dean et al., 2016; Dresel et al., 2018; Hamilton et al., 2018). For example, Brown et al. (2015) found that, at regional scales, streamflow was mainly driven by climate variability, rather than land use and land use change. Likewise, Dean et al. (2016) found that the streamflow in a catchment forested with a *Eucalyptus* plantation did not change considerably when compared to a catchment covered by a pasture for grazing. Contrastingly, when studying data from 26 catchments around the world, Farley et al. (2005) found that afforestation could reduce the streamflow by 50% in catchments where the streamflow represents less than 30% of precipitation or dry streams where streamflow is 10% of precipitation. Similarly, Jackson (2005) analysed approximately 504 annual catchment observations and concluded that afforestation decreased streamflow after a few years of planting, and also caused soil nutrient scarcity.

The contrasting results from different climates and regions makes it challenging to define unified management practices and water regulation policies. Among the factors cited as being responsible for the lack of agreement within the results are the small percentage of land-use change (less than 20% of the catchment), and lack of study sites located in intermittent streams and low precipitation areas (< 800 mm/year) (Brown et al., 2005), and limited information on water yields at a seasonal scale (Dye, 2013, 2000). Additionally, paired catchment analyses usually investigate mean annual changes in the water yield, which result in less information about the effects of afforestation on monthly and seasonal time scales (Brown et al., 2015; Dresel et al., 2018). The changes occurring at the seasonal and intra-annual scale are important since rainfall frequency, weather conditions, management cycle, and practices are relevant site-specific parameters with high variability within a year (Dye, 2013). Changes in these parameters can alter the ecosystem dynamics and, consequently, streamflow (Adelana et al., 2014).

As the demand of water for productive plantations is growing over time, the monitoring of hydrological variables at relatively high temporal and spatial resolutions is increasing in importance (Dean et al., 2016; Dye, 2013). For example, during the first years after plantation establish-

ment, studies found considerable variability in water yield. During this stage there is more recharge and soil exposure, given the shallow roots and shorter trees (Ferraz et al., 2019; Forrester et al., 2010a; Liu et al., 2017), which can result in more streamflow. Other studies have reported variable plantation water use due to different soil conditions, geological and topographical features (Dresel et al., 2018), and right after tree harvesting (Rodrigues et al., 2011). The length of the rotation has been also evaluated, and shorter rotation periods (i.e. 6-7 years in Brazilian *Eucalyptus*) may not allow soil water recharge and nutrient cycling (Christina et al., 2016), and probably result in high tree water use at any stage (Almeida et al., 2007; Hubbard et al., 2010).

The dearth of experimental observations on plantations considering site-specific studies, seasonal and inter- and intra-annual differences in catchment dynamics makes it difficult to estimate and predict the relationship between land use and water resources (Dean et al., 2016). Therefore, extensive research on plantation dynamics is required to fully understand the impact of afforestation on water resources (Adelana et al., 2014; Dye, 2013).

2.2 Commercial plantations in Australia

Australia is mostly a semi-arid country, with limited water availability. This limitation requires an investment into researching sustainable management practices to allow economical growth without harming surface and groundwater resources (Benyon et al., 2006; Greenwood, 2013). In some parts of Australia, native deep-rooted vegetation was cleared to open space for crop production and pastures (Benyon and Doody, 2004), resulting in an increase of water in the ecosystem (when compared to the native vegetation), leading to soil salinization due to shallower water tables (Daneshmand et al., 2020; Rengasamy, 2006). As a consequence, in addition to the industrial and economical incentives, commercial plantations were encouraged in an attempt to solve salinization problems. However, after a long drought period, known as the Millennium Drought, water availability issues were prioritized over the salinity problems (van Dijk et al., 2013).

Until the early 1990s, most of the *Eucalyptus* were harvested from native forest (Acuña et al., 2018; Harper et al., 2014). As demand for pulp increased along with the incentives to expand plantation areas, large areas of *E. globulus* and *E. nitens* were established between the 1990s and 2010 (Benyon and Doody, 2004). The latest plantation statistics show that the total commercial plantation area in Australia is 1,933,400 hectares, with Victoria having the largest area (418,500 hectares) (Figure 2.1). The *E. globulus*, known as the Tasmanian blue gum, is the most planted hardwood specie and represents 50% of all hardwood plantations, while the radiata pine is the most planted softwood tree (75% of all softwood plantations) (Downham and Gavran, 2020).

Australia total plantation area NPI regions, 2019–20

Total plantation area (ha)

- < 25,000
- 25,001–50,000
- 50,001–100,000
- 100,001–200,000
- 200,001–400,000

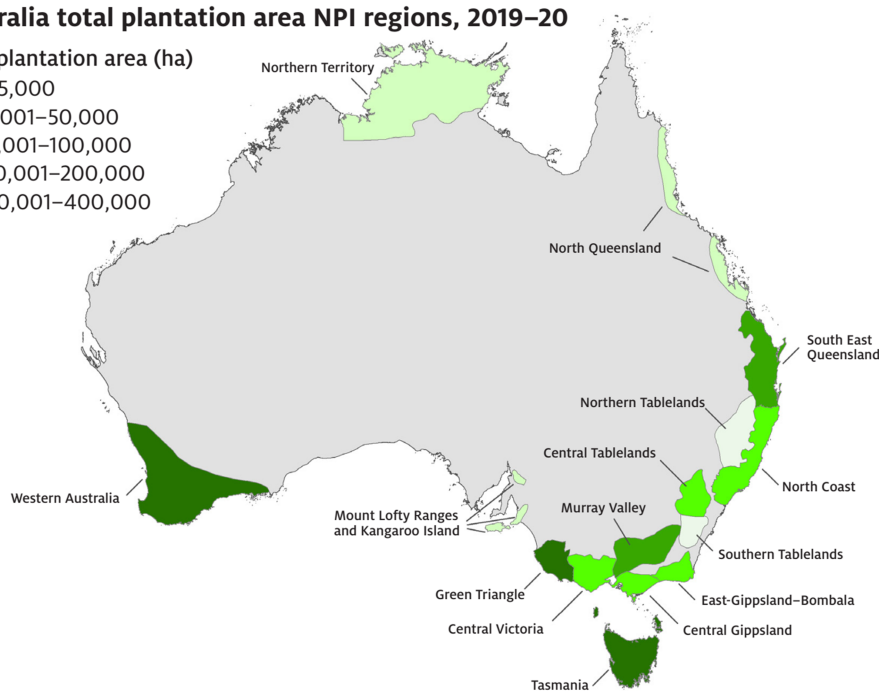


Figure 2.1: Map of the National Plantation Inventory (NPI) regions for 2019-20. Retrieved from Downham and Gavran (2020).

Despite the majority of commercial plantations being located in Victoria, the state of South Australia was the first to consider commercial plantation as a water interception activity. This led to the introduction of the first Australian plantation water policy in 2011 (Dye, 2013; Greenwood, 2013). This initiative was mainly motivated by the scarcity of water resources in the state, where most of the water comes from groundwater, with limited superficial water (Dye, 2013). Australia was the second country in the world to regulate water used by forests, only behind South Africa (Gush et al., 2002). Greenwood (2013) provides a comprehensive overview of the development of the Australian policy, including a description of the water accounting models used as a baseline for the South Australian policy. Considering the concern with groundwater resources, the South-Australian models assess the effects of forestry on the groundwater recharge, defined as the water entering the water table from annual rainfall after evapotranspiration and run-off are accounted for. The legislation is applied on a interception rate of groundwater recharge, calculated as a annualised average over the management cycle. In 2006, the legislation was reviewed and started to include direct groundwater extraction, as there was evidence that trees could use groundwater (Benyon et al., 2006).

In the reviewed legislation, direct groundwater extraction happens when water tables are less than 6 m deep and after canopy closure is reached. The interception rates are assumed 78% per year, as an annualised average applied considering an 11 years management cycle. Interception rates are negative during the first year, reflecting an agreed allowance for recharge

(120%) compared to dryland pasture reference levels, 20% on the second year, 60% on the third year, and 100% starting on the fourth year, when canopy closure is assumed (Figure 2.2). This approach limits the estimation of the plantation impacts on the regional water resources, since applying an annualised average during the entire management cycle may not reflect a realistic water use by the trees and result in underallocation or overallocation of resources. In addition, the South Australian forestry policy was based on a limited dataset, with a few monitoring sites and limited monitored period (Benyon et al., 2009), which introduced uncertainties in the results used to provide the policy guidelines (Greenwood, 2013).

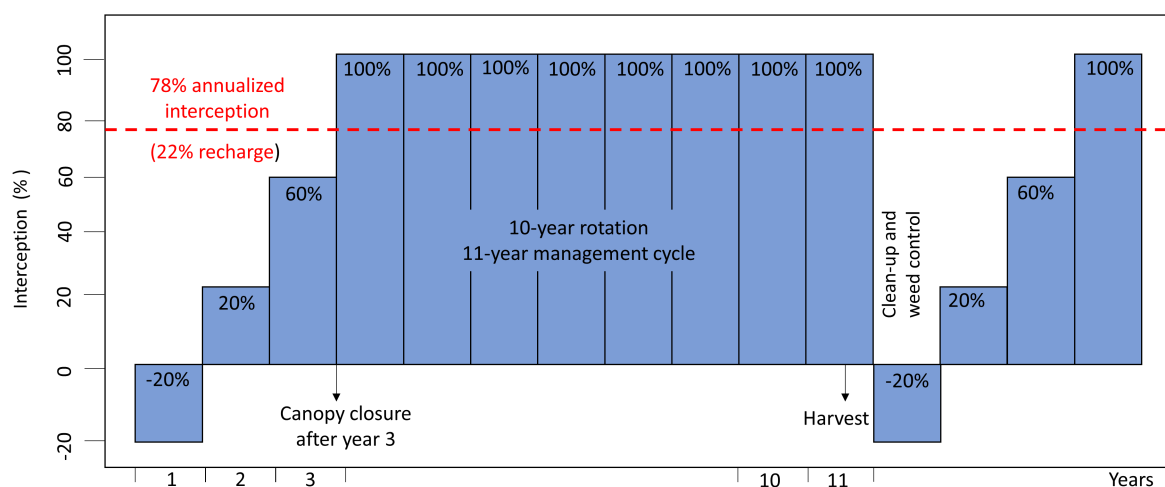


Figure 2.2: Annualised groundwater recharge reductions for blue gum plantations due to interception of recharge, defined as the water entering the water table from remaining annual rainfall, after evapotranspiration and run-off are accounted for, according to the 2006 South Australian model. Negative interception reflects an agreed allowance for recharge (120%) compared to dryland pasture reference levels. Modified from Greenwood (2013).

Considering that planning the allocation of water licenses for plantation activity depends on modelling, the management of commercial plantations and lessen water conflicts between landowners and the government require efficient modelling of the hydrological effects of forestry on the water resources (Dye and Versfeld, 2007; Greenwood, 2013; Gush et al., 2002). Model accuracy can be critical to not only protect the regional water resources, but also assure that the landowners are paying a fair and well based value for water and that licenses are distributed in an efficient way (Benyon et al., 2009; Benyon and Doody, 2004). As a consequence, the study of plantation water use and related ecosystem scale variables (e.g., evapotranspiration, interception, streamflow, water use efficiency) is required to better understand the variability and magnitude of plantation establishment impacts on the water resources (Dean et al., 2016; Scott, 2005), which will, in turn, benefit the water license allocation.

The current plantation management practices aim to achieve maximum productivity through successive plantings and harvests. Since plantation productivity is known to decrease with stand age (Bergeron et al., 2008; Clark et al., 2004; Ryan et al., 2004, 2010), rotations prioritize

maintaining fast growing trees such as *Eucalyptus globulus* and *Eucalyptus grandis*. However, high productivity can come at the expense of higher water use. When enough water is available to maintain high transpiration rates, it leads to considerable stem growth over the year, which makes *Eucalyptus* efficient trees (Cristiano et al., 2020; Dye, 2000).

Most plantation species, including blue gum trees, can adapt to the wide ranges of environmental conditions found in Australia (Drake et al., 2009), such as different geology (Dean et al., 2016), precipitation regimes (Bleby et al., 2012), temperature (Griebel et al., 2020), and salinity (Barrett et al., 2005; Beverly et al., 2005). Specifically, plantation evapotranspiration, interception, and growth can be highly variable over time and space (Almeida et al., 2007; Forrester et al., 2006). The non-linear relationship between stem growth and water use indicates that for a complete and accurate study of plantation characteristics, knowledge of the whole rotation period (or simultaneous measurements for different age classes) is necessary (Chan et al., 2018; Ma et al., 2019; Skubel et al., 2015). Therefore, to fully understand how plantations affect water resources in the long-term, information on water use during the entire management cycle, including the period before canopy closure, needs to be taken into account (Migliavacca et al., 2021).

2.3 Water and carbon fluxes in productive ecosystems

One of the main consequences of the changes in land use, such as replacing pastures with forests, is the increase in evapotranspiration from the landscape, as trees tend to transpire more water (Almeida et al., 2007; Stape et al., 2004). This can change the components of the catchment water balance and, at the same time, it alters the amount of carbon assimilated by the trees, which affects the productivity of the ecosystem. This productivity is defined as the amount of carbon assimilated against the amount of water used by the ecosystem. The impacts of afforestation or deforestation can be quantified by the ecosystem water and carbon fluxes, and the variables controlling them, such as precipitation, solar radiation, vapour pressure deficit (VPD), and air temperature (Pastorello et al., 2020).

Water, energy, and CO₂ fluxes can be measured simultaneously with the eddy covariance (EC) technique (Baldocchi et al., 2018; Baldocchi, 2003; Cleverly et al., 2020; de Araújo et al., 2010; Granier et al., 2008; Mendes et al., 2020), which can provide high temporal resolution measurements of energy, water, and CO₂ exchange at the ecosystem scale through the use of fast response instrumentation (Burba and Anderson, 2007). The technique is based on the turbulent exchange of energy and mass between the surface and the atmosphere (Baldocchi, 2008). Even though performed at a point, EC measurements can be considered to represent spatial averages for a larger area, referred to as "footprint". This area is a function of measurement height, wind speed and direction, surface roughness and atmosphere stability, which

also means that the measurement height must be representative of the entire footprint surface (Burba and Anderson, 2007).

Many studies have measured CO₂ and water fluxes using the EC technique across different biomes around the globe. A global network, the FLUXNET project (<http://fluxnet.ornl.gov/>) is integrated by EC sites monitoring the land-atmospheric gas exchanges (Pastorello et al., 2020). EC sites in Australia are part of the OzFlux (<http://www.ozflux.org.au/>) within the Terrestrial Ecosystem Research Network (TERN) (Beringer et al., 2016). EC measurements have enabled detailed analysis of processes, relating plant physiological processes, water fluxes and atmospheric drivers. Additionally, the EC technique provides measurements of different components to generate a complete water balance (Baldocchi, 2008; Baldocchi et al., 2018).

At the ecosystem scale, EC measurements of latent heat flux (LE) can be used to derive evapotranspiration. Additionally, one of the main outputs from an EC system is the carbon exchange between the ecosystem and the atmosphere, which is denominated the Net Ecosystem Exchange (NEE). NEE is the net flux between the CO₂ from photosynthetic uptake (Gross Primary Production - GPP), and ecosystem respiration (ER), which is composed of the respiration by plants, from decomposition by soil microbial components, and root respiration (Anthoni et al., 2002; Granier et al., 2008; Luo and Zhou, 2006) (Figure 2.3). NEE is the measured variable, with GPP and ER being estimated by the application of mathematical models, which are usually based on light and temperature thresholds (Barr et al., 2013; Foken et al., 2012; Lasslop et al., 2010).

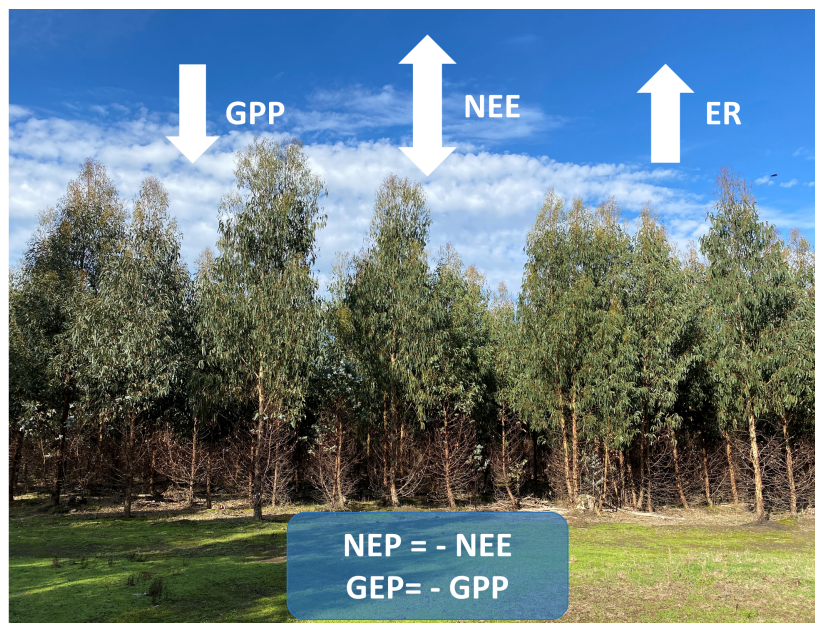


Figure 2.3: Schematic view of the NEE partition between GPP and ER.

The micrometeorological convention for fluxes is relative to the atmosphere, i.e. positive fluxes represent a gain to the atmosphere and negative fluxes a loss. The ecological convention is re-

lative to the ecosystem, i.e. positive (negative) fluxes represents ecosystem carbon gain (loss). The ecological convention is usually applied for annual budgets, with the terms Net Ecosystem Production (NEP), defined as $NEP = -NEE$, and Gross Ecosystem Production (GEP) defined as $GEP = -GPP$ (Chapin et al., 2006, 2012).

NEE only includes carbon transferred from and to the atmosphere, thus not including other transfer pathways, such as aquatic exchange of dissolved organic and inorganic carbon. However, since other carbon transfers can be considered small in the majority of ecosystems and scenarios, NEE is a useful approximation of the total ecosystem carbon balance (Chapin et al., 2012; Luo and Zhou, 2006). Regarding plantation management, GPP can be a measurement of plantation productivity and wood production, since it gives the gross carbon uptake of the ecosystem, making it a strategic variable (Burba and Anderson, 2007). The magnitude of NEE, GPP, and ER responses can vary for different sites, species, and stand age (Baldocchi et al., 2021; Cleverly et al., 2020).

Analysing the variables measured with the EC technique over different sites and land uses can assist in the understanding of the key hydrological components of commercial plantations, and the impacts it may cause over a long term (Baldocchi et al., 2018). Year to year changes in structural and functional characteristics of an ecosystem may explain a significant portion of the evapotranspiration and carbon uptake observed. Therefore, EC measurements may be accompanied by measurements of LAI, diameter at breast height (DBH), and stand height, for example. Nevertheless, the EC measurements allow the development and application of models to quantify water use, forest productivity, and investigate tree traits (Almeida et al., 2007, 2010; Christina et al., 2016).

2.3.1 Drivers of water and carbon fluxes in plantations

The amount of water used and carbon assimilated by trees can provide insights about the plantation ecosystem dynamics (Baldocchi, 2008; Baldocchi et al., 2018; Pastorello et al., 2020). Water use and carbon assimilation are controlled by physiological variables such as the leaf area index (Irvine et al., 2004), plant functional type (Cabral et al., 2011; Campoe et al., 2020), and environmental variables, including solar radiation (van Gorsel et al., 2013), air temperature (Brümmer et al., 2012; Wardlaw, 2022), and water availability (Calder, 2007). Given the complexity and diversity of these drivers, measurements of carbon and water fluxes can vary considerably in space (site-specific to regional scales) and time (intra- and inter-annual periods) (Cleverly et al., 2020; Eamus et al., 2013).

In semiarid ecosystems, such as the majority of Australia, carbon and water fluxes are commonly correlated with precipitation (Baldocchi, 2008; Mendes et al., 2020). In conjunction, variables modulated by precipitation, such as temperature, VPD, and soil moisture, also impact the carbon and water fluxes (Jiang et al., 2020). As a result, plantations in semiarid regions can

behave as a sink or source of carbon depending on precipitation, flipping from being a sink to a source, and vice-versa (Bracho et al., 2012; Gonçalves et al., 2017; Rodrigues et al., 2011). Additionally, the occurrence of disturbances (i.e., droughts, insect attacks, heat waves, and land use change) can shift the whole ecosystem to an overall carbon source (Cristiano et al., 2020; da Silva et al., 2015; Wardlaw, 2022). This is explained by the decreases in GPP, which might be accompanied by increases in ER from different inputs, such as litter, harvesting, and fertilization. This might surpass GPP and shift the NEP (Almagro et al., 2009; Brümmer et al., 2012; Reichstein et al., 2005a). Temperature can be also a main constraint on the NEP, since it is the main driver of the ER. Increases in temperature may decrease local soil moisture and increase evaporation, affecting both NEP and ET (Marcolla et al., 2011; Pereira et al., 1986, 2007; Pita et al., 2013). High temperatures are usually found during drier years, which are associated with more radiation, and increases in photosynthesis until high VPD and low soil moisture limit carbon uptake due to stomatal closure, which reduces photosynthesis (Pita et al., 2013; Renchon et al., 2018). In productive ecosystems, the amount of rain during spring, a period of high productivity for the plants, can be also an important factor controlling NEP (Chan et al., 2018; Ma et al., 2019; Ryan et al., 2010; Sun et al., 2010).

Despite a strong correlation, water availability not always leads to a carbon sink. Wetter periods followed by decreases in solar radiation may reduce photosynthesis and, as a results, the NEE can become positive (Eamus et al., 2013). For example, in a temperate *Eucalyptus* forest in NSW, NEE was mostly correlated with incoming solar radiation, with precipitation negatively correlated with NEE on a scale of 4-8 days due to enhanced cloud cover, which reduced radiation (van Gorsel et al., 2013). Water availability not only influences the NEP and ET, but can modify above and below ground carbon allocation, favoring roots or stem development (Dye, 2000). Mature trees usually present an already developed root system, resulting in more growth during dry seasons (Ryan et al., 2010; Stape et al., 2004). Contrarily, younger stands may allocate more carbon into developing their root system in order to get access to water in deeper soil layers and survive drier periods (Moroni et al., 2003).

Changes in stand structure and ecosystem traits can also drive the dynamics of water and carbon fluxes in plantations (Bracho et al., 2012; Chan et al., 2018; Nosoetto et al., 2020). Variations in LAI, for example, affect the photosynthetic capacity of the plant, which in turn affects the carbon uptake and ET (Baptista et al., 2018; Battaglia et al., 1998; Binkley et al., 2010). Other functional traits, such as the size and shape of the leaves, alter the dynamics of light capture and, thus, affect the carbon assimilation (Drake et al., 2018; Whitehead and Beadle, 2004). Therefore, forest growth causes variability in the NEE and ET (Christina et al., 2016; Stape et al., 2004). Fast growing species, such as plantation trees, are associated with increasing LAI and height as the stand develops, promoting a fast increments in carbon assimilation (Forrester et al., 2010a,b). The water uptake by the expanding root system and greater leaf area may also increase water use with tree growth (Benyon and Doody, 2015; Benyon et al., 2006).

For plantation trees, productivity is an important variable, given the importance of maximizing the amount of carbon sink against the amount of water used (Almeida et al., 2010).

2.3.2 Water use efficiency of plantations

Continuous measurements of NEE, and the subsequent partition of NEE to GPP and ER, allow estimations of the ecosystem water use efficiency (WUE). WUE is the ratio between the net production of carbon stocks and the amount of water consumed by the trees to produce these stocks. At the ecosystem level, WUE is defined as the ratio of gross ecosystem production (GEP) to evapotranspiration (ET) ($WUE = GEP/ET$) (Dye, 2000). The WUE represents an important ecophysiological variable reflecting the relationship between ecosystem water use and productivity (Baldocchi et al., 2021).

The WUE also assesses the ecosystem response to climate variability (Cabral et al., 2020). Seasonal and inter annual variability in environmental variables, including soil water supply, might impact the carbon balance by modifying the photosynthesis rate, which affects the stomatal conductance and the evapotranspiration (Jassal et al., 2009; Tfwala et al., 2019). For example, Tong et al. (2014) concluded that, for a mixed plantation in China, WUE decreased considerably during a vigorous growing season, due to strong solar radiation and higher VPD, which in this case increased evapotranspiration at a higher rate than GPP. In contrast, for a *Eucalyptus globulus* site in Brazil, Reis et al. (2019) discussed the highly effective stomatal regulation of blue gum trees, resulting in a maximum WUE even during the warm and drier season.

The stomatal conductance reflects how plants respond to changes in environmental variables, such as humidity, soil moisture, and light, thereby influencing the amount of water used and carbon assimilated by trees (Dye, 2000; Ma et al., 2018). Through stomatal responses, the WUE indicates plant water use strategies under different scenarios of water availability and distinct environments (Hubbard et al., 2010; Sun et al., 2010). For example, reductions in stomatal conductance can work as a defense mechanism to avoid water stress. As a result, water losses are avoided but at the same time CO₂ supply is limited. Therefore, plant growth, biomass allocation and evapotranspiration rates are strongly influenced by the WUE (Chapin et al., 2006, 2012).

The WUE is also modulated by species, plant functional type, stand age, and disturbances. For example, during the early years of a blue gum plantation studied by White et al. (2014), WUE decreased as the soil water deficit increased, with more carbon being allocated to roots, and less to wood. Contrarily, when studying mature stands, Griebel et al. (2020) registered an increase in WUE in response to water stress; this was explained by stomatal closure and deeper roots, as supported by other studies (Li et al., 2012; Pereira et al., 1986; Tong et al., 2014). However, for all these studies, WUE ultimately decreased during extreme drought stress.

Management practices, such as fertilization and irrigation, can influence WUE by increasing GPP due to above ground stem increment. For example, when studying the carbon allocations in a *Eucalyptus* plantation, Ryan et al. (2010) found that the annual fraction of GPP used for below ground (roots and stem) did not change in irrigated stands at the same time when the fraction to above ground carbon increased. In a different study, Ryan et al. (1996) identified that the combination of fertilizers and irrigation decreased the below ground allocation. Recent studies indicate that managing plantations for maximising their above ground growth can also result in a maximum WUE, given that increases in water use are offset by a greater increase in above ground carbon allocation (Stape et al., 2004; White et al., 2014). When comparing a native forest to commercial *Eucalyptus globulus* stands, White et al. (2021) found that while blue gum stands transpire more, they grow at a much faster rate when compared to native stands, thus having higher WUE. Similarly, Stape et al. (2004) investigated the WUE for irrigated stands and found a higher WUE during wet and drier years, when compared to control stands, with a 52% increase in wood production versus a 32% increase in water use.

Stand age and development stage are also factors that influence on the plantation WUE. Studies have found increasing WUE as stands grow and develop as a result of larger increases in GPP than in ET, as a consequence of an expanding LAI, sapwood area, and root system (Chan et al., 2018; Irvine et al., 2004; Jassal et al., 2009). When trees are very young and canopies are sparse, soil evaporation can be a major water flux and contribute significantly to ET. Additionally, reduced stand LAI may favour the growth of understory vegetation, since sparser canopies intercept less light and water than closed canopies. Understory vegetation might increase the ecosystem GPP, but it also has the ability to use water with low stomatal control, usually resulting in more water being transpired, generating more ET than increments in GPP (Forrester et al., 2010b; Irvine et al., 2002; Ntshidi et al., 2021; Rodrigues et al., 2011). After reaching canopy closure, WUE may decline following decreases in GPP, due to an overall decline in LAI and growth rates (Almeida et al., 2007). For Forrester et al. (2010a), WUE and growth peaked around 5 years for blue gum stands, and then declined with stand age.

The different responses in WUE when comparing climatic variability and differences in management highlight the need to evaluate WUE in order to optimize productivity while minimizing the water use, taking into account tree physiological dynamics and species characteristics. Optimum management practices need a good understanding of the effects of climate on the growth and WUE of plantations (Forrester et al., 2010b; Hubbard et al., 2004).

2.3.3 Water use and carbon assimilation in young plantations

Plantation trees experience changes in their structure and physiology during the entire rotation. Young trees have been found to display these changes in a more rapid way than mature trees and well established forests (Chan et al., 2018; Li et al., 2012). Therefore, as trees age and

develop, there is also a change in the dynamics of water use and carbon assimilation (Chan et al., 2018; Clark et al., 2004; Coursolle et al., 2012).

A number of studies were dedicated to evaluate the water, carbon and energy balance of mature forests (Battaglia and Sands, 1997; Law et al., 2001; Nosetto et al., 2005) or forested stands that underwent productivity declines as they reached older ages (Almeida et al., 2007; Hubbard et al., 2010; Law et al., 2001; Ryan et al., 2004). However, the monitoring of water and carbon fluxes in young and newly established tree stands is recognized to be sparse in the literature, with a limited number of studies monitoring fluxes during the first years after plantation establishment (Anthoni et al., 2002; Bergeron et al., 2008; Chan et al., 2018; He et al., 2012; White et al., 2021). This means that the dynamics of carbon assimilation and water uptake in young stands are not well-known. Table 2.1 summarizes the findings of several studies on carbon assimilation and water use that are available in the literature.

A common aspect highlighted by some of the studies listed in the Table 2.1 was the predominance of the sensible heat flux over the latent heat flux during the monitoring period (Chan et al., 2018; Ma et al., 2018). This was explained by the sparse canopy of the sites, since the plantations had not reached canopy closure yet. Latent heat flux dominated during the growing season, when enough soil moisture was present. Alternatively, other studies did not register much variability in the partition of the sensible and latent heat flux over time, but registered changes in the understory vegetation of the plantation (Forrester et al., 2010a; Irvine et al., 2002; Ntshidi et al., 2021). The reduced LAI of younger trees facilitates the growth of understory vegetation, which usually have substantial fluxes of carbon and water. As trees develop and the LAI increases, the understory contribution reduces considerably and the trees become the main contributor to the ecosystem fluxes. For a pine plantation in early developmental stage, Bracho et al. (2012) found that carbon assimilation was majorly driven by increases in LAI.

Younger trees are usually a source of carbon during the first few years after establishment. The age of transition from a carbon source to a sink is quite variable even among stands from the same species due to variable climate and site-specific aspects (i.e., soil type, disturbance history, and land use) (Bjarnadottir et al., 2009; Chan et al., 2018; Coursolle et al., 2012; Peichl et al., 2010; Sun et al., 2008). During the first few years after plantation establishment the ecosystem usually releases more carbon through ER than what is assimilated by photosynthesis (GPP) (Anthoni et al., 2002; Bracho et al., 2012). This was observed in the site described in Granier et al. (2008), who concluded that more than half of the assimilated carbon in a plantation in France was lost by the respiratory processes. Similarly, for a site located in Iceland, Bjarnadottir et al. (2009) concluded that the annual variations in NEE were apparently more linked to differences in ER due to decomposition of organic matter.

The prevalence of ER over GPP soon after plantation establishment was highlighted in Chan et al. (2018), who measured NEE for a pine plantation forest at the beginning of the rotation. In

their study, the site was a source of carbon during the first 4 years. High temperatures during the dryer periods drove increases in ER, which was larger than carbon assimilation, turning the site to an overall source. Contrastingly, the sites of Bergeron et al. (2008) and Coursolle et al. (2012) registered lower values of NEE since plantation establishment, due to a low residual soil carbon pool, which resulted in considerably lower ER. The low residual soil carbon enabled the sites to become sinks in a shorter time interval, highlighting how site-specific aspects can change the dynamics of carbon fluxes. For example, for the same species and with both sites located in Canada, the site described in Coursolle et al. (2012) became a sink after only 2 years, versus 4 years for Chan et al. (2018).

The dynamics of NEE can change dramatically over the years, due to the influence of tree age, structure and the effect of climate on growth (Cabral et al., 2011; Campoe et al., 2020). In addition to management practices, the climate of the region strongly influences the potential carbon assimilated during the first years of development. Since young trees have a shallower root system, they depend on soil moisture from the shallow layers of soil, which is mainly driven by precipitation (Zha et al., 2009). As a result, young stands are more vulnerable to water stress (Anthoni et al., 2002). In particular, Zha et al. (2009) identified larger variability for variables monitored for the younger stands, meaning that young trees can display more dramatic responses due to changes in temperature and precipitation, when compared to more mature trees.

The reviewed studies emphasized the high spatial and temporal variability of the carbon fluxes and water use among different species. In particular, the studies highlighted the need for contribution in the monitoring of carbon and water fluxes over diurnal, seasonal and annual scales for the entire cycle, since only a few studies have examined how age and growth influence the ecosystem-scale energy balance, transpiration rates, and net carbon uptake.

Table 2.1: List of literature on young and developing plantations and a summary of their findings.

Reference	Species	Location	Age	Findings
Anthoni et al. (2002); Law et al. (2001)	<i>Pinus ponderosa</i>	Central Oregon, USA	15 years old	The ratio ER/GEP varied seasonally, and ranged from 0.4 to 1.45
Bjarnadottir et al. (2009)	Siberian larch (<i>Larix sibirica</i> Ledeb)	Eastern Iceland	12 - 14 years	Sink after 12 years. Respiration and decomposition were the main driver for NEE variability
Bracho et al. (2012)	Slash pine (<i>Pinus elliottii</i>)	Gainesville, Florida, USA	1 - 9 years	Sink after 4 years. Drought had a much stronger impact on GEP than on ER, resulting in a clear reduction in NEP
Cabral et al. (2011)	<i>E. grandis</i> x <i>E. urophylla</i>	Sao Paulo, Brazil	2 - 4 years	Source or sink behaviour (NEP) was mainly influenced by changes in GEP due to rainfall variability
Chan et al. (2018)	White pine (<i>Pinus strobus</i> L.)	Southern Ontario, Canada	1- 14 years	Sink after 5 years, subsequent source years related to dry years and droughts
Coursolle et al. (2012)	White pine (<i>Pinus strobus</i> L.)	Ontario, Canada	Young 1- 15 years	Source up to 17 years. LAI was the main factor affecting GEP, ET, and NEP of young stands
Forrester et al. (2010a)	<i>Eucalyptus globulus</i>	Ballarat, Victoria, Australia	2, 4, 5, 6, 7 and 8 years	Transpiration and LAI declined for older stands (5-7 years), consequently, WUE also declined
Granier et al. (2008)	European beech (<i>Fagus sylvatica</i> L.)	North-eastern France	29 - 40 (+/- 5) years	NEP correlated with tree growth. Drought and management explained most of the variability in fluxes and growth

Table 2.1: List of literature on young and developing plantations and a summary of their findings.

Reference	Species	Location	Age	Findings
Harper et al. (2014)	<i>Eucalyptus globulus</i> , <i>Eucalyptus occidentalis</i> , and <i>Pinus radiata</i>	Corrigin, Western Australia	1 - 6 years	Marked differences in tree response to slope across the site. Increasingly WUE as tree aged
Irvine et al. (2002)	<i>Pinus ponderosa</i>	Oregon, USA.	14 years	CO ₂ fluxes in young stands correlated with LAI and root development
Krishnan et al. (2009)	Douglas-fir	East coast of Vancouver Island, BC, Canada	3-7 years	Stand-age effects on carbon fluxes were much higher than that of interannual variability
Ntshidi et al. (2021)	Orchard	Koue Bokkeveld, South Africa	5- 7 years old	Dense understory contributed to almost 40% of ET of young orchards
Ma et al. (2018)	<i>Pinus tabuliformis</i>	Nothern China (Beijing, China)	*	Seasonality in ET was controlled by biological factors and water availability
Marcolla et al. (2011)	<i>Festuca rubra</i> (L.)	Viote del Monte Bondone, Italian Alpes	cut annually	In the warmest and driest years the ecosystem was a significant source of CO ₂
Nosetto et al. (2005)	<i>Eucalyptus grandis</i>	Western coast of the mid-Uruguay river in Argentina	1 - 9 years	ET changes with age showed that tree water use rose at a steady state until 4–5 years of age, having a slow increase afterwards
Reis et al. (2019)	<i>Eucalyptus grandis</i>	Mato Grosso do Sul State, Brazil	1-2 years	Young eucalypt exhibited higher photosynthetic capacity, particularly during the dry season, which is likely associated with growth maintenance

Table 2.1: List of literature on young and developing plantations and a summary of their findings.

Reference	Species	Location	Age	Findings
Rodrigues et al. (2011)	<i>Eucalyptus globulus</i>	Espirra Estate, Portugal	before (8 - 12 years old trees) and after a felling (1 - 3 years old trees)	The young eucalypt coppice behave as a carbon source in the first seven months of the new rotation. Increasingly WUE with tree growth
Skubel et al. (2015)	<i>Pinus strobus</i> L.	Ontario, Canada	11 years	ET was most conservative in the youngest forest, which led to an increase in WUE when compared to mature stands
Sun et al. (2010)	Loblolly pine	North Carolina, USA	3-5 years	ET/P was 0.66 for 4 years old stands compared to 0.88 for 16 years old stands
Thornton et al. (2002)	<i>Pinus ponderosa</i>	California, EUA	1-10 years	Ecosystem behaved as a carbon source followed by strong and gradually diminishing sink after harvesting
Vertessy et al. (2001)	<i>Eucalyptus regnans</i>	Melbourne, Australia	15 years	Total annual ET declines from 1371 mm at age 15 years to 911 mm at age 240 years, following decreases in LAI
Vickers et al. (2012)	<i>Pinus ponderosa</i>	Central Oregon, USA	16 years	Annual NEE 3 times smaller when comparing young to mature stands. This is correlated with the larger LAI for mature stands
Zha et al. (2009)	Jack pine (<i>Pinus banksiana</i>)	Saskatchewan, Canada	2-90 years	Following clear cutting, site site behaved as slight sink at year 10 and strong sink at year 30. NEE followed increases in LAI

2.4 Modelling plantation water use

Modelling plantation water use is important to guide policy and management decisions, also allowing the exploration of different afforestation scenarios (Almeida et al., 2007; Bonan et al., 2014). Models that can accurately simulate the complexity of plantation trees, with adequate data requirements, are recommended for this task (Greenwood, 2013).

A large number of studies have been conducted to model the impact of land use, including afforestation, on the water resources and have shown such changes to be important (Adelana et al., 2014; Almeida et al., 2010; Azarnivand et al., 2020; Dresel et al., 2018; Miehle et al., 2006). There are different approaches to model vegetation water use and its impact on water resources. This section will discuss a variety of approaches, from simpler models, such as the Zhang curves, to process-based hydrodynamic models. Table 2.2 presents some key studies on the different model approaches discussed in this review.

2.4.1 Zhang curves

One of the first efforts in assessing the hydrological role of vegetation resulted in the so-called Zhang curves (Zhang et al., 1999, 2001), which were derived from data obtained in catchment water balance studies and paired-catchment studies. The Zhang curves are based on a relationship proposed to predict the effect of vegetation changes on evapotranspiration. This relationship yields a dimensionless function and it can be used to calculate the mean annual actual evapotranspiration when annual rainfall and potential evapotranspiration are known. The Zhang curves were the basis for estimating the impact of forest and land-use change on streamflow in a number of studies, including applications in the Australian Government, policy organisations, and research publications (Bren et al., 2006; Brown et al., 2006; Keenan et al., 2004; Zhang, 2004; Zhang et al., 2001, 2003, 2007).

The Zhang curves were developed using data from catchments where slopes were gentle and the soil was relatively thick. Detailed information regarding vegetation types was not available, so vegetation was classified as herbaceous plant, herbaceous plants and trees, and forest. The catchment size was variable, including areas from 1 km² to 600,000 km² (Zhang et al., 1999, 2001).

The Zhang curves have the advantage of being a practical tool, usually requiring data already available and only using two parameters, which are fixed. They have potential uses in catchment-scale studies of land-use change, such as afforestation and deforestation. However, one of the main limitation of this method is that it is only reliable for catchments with average annual precipitation greater than 1000 mm. In a technical report, Greenwood (2007) describes the discrepancies between measured South Australian data and theoretical data from the Zhang

curves (Zhang et al., 1999, 2003). The theoretical Zhang curves did not show strong agreement with measured data from any Australian catchment with mean annual rainfall less than approximately 1000 mm/year, which includes the majority of Australia. Under lower annual rainfall, it underestimates evapotranspiration in forest, mixed vegetation, and pasture, resulting in overestimated predictions of runoff (Dresel et al., 2018). Additionally, since the method is based on mean annual data, it should not be used to explore inter-annual variability, as stated in the original work of Zhang et al. (1999). For values of the parameters, the Zhang curves also do not satisfy the water balance, as noted by Daly et al. (2019). Therefore, the application of the Zhang curves can underestimate the impacts of afforestation and its implications for water resource management. As consequence, resources can be over-allocated, with effects for all downstream users and the environment (Greenwood, 2007).

2.4.2 Water use models in forest growth models

Process-based forest growth models have become widely used as a means of predicting the growth of plantations and native forests in Australia and South Africa (Dye, 2000; Dye et al., 2004). These models estimate forest physiological and environmental factors to calculate their influence on stand growth. Usually, these models estimate the GPP from photosynthetic active radiation and use simple empirical relationships to predict forest growth and productivity. The empirical relationships are derived from measurements and experimental data collected on forests and plantations during a considerably long period. Process-based models vary in complexity and scale of application (Battaglia and Sands, 1997; Miehle et al., 2006; Sands and Landsberg, 2002), but are usually applied at seasonal and annual resolutions (Feikema et al., 2010).

The 3PG (Physiological Principles in Predicting Growth) forest growth model was developed by Landsberg and Waring (1997) and requires relatively few input data. It has been variously described as process-based, mechanistic, hybrid, and semi-empirical (Sands and Landsberg, 2002). Much of the focus of the development of 3PG, and indeed other forest growth models in the past, has been on their use for predicting the growth of commercial plantations (Almeida and Sands, 2016; Almeida et al., 2007), and relatively little emphasis has been given to validating or improving predictions of plantation water use. The 3PG model has been parameterized for different plantation species, including *Eucalyptus globulus* (Sands and Landsberg, 2002) and *Eucalyptus grandis* (Almeida et al., 2004), but it has shown poor results before canopy closure and during early canopy development (Dye, 2001; Dye et al., 2004).

An updated version of the model, 3PG+ was designed to be coupled to the Catchment Analysis Tool (CAT) (Beverly, 2007; Beverly et al., 2005). CAT is a modelling framework based on the one-dimensional crop model PERFECT (Productivity, Erosion and Runoff Functions to Evaluate Conservation Techniques) (Littleboy et al., 1989). CAT includes a water balance model, which

allowed 3PG+ to estimate a daily multi-layered soil water balance, runoff from rainfall, and soil evaporation. The coupling of 3PG+ to CAT enabled the simulation of plantation water use at a daily time step and, at the same time, the simulation of dynamic forest growth. When applying 3PG+ in CAT, Feikema et al. (2010) concluded that the model can satisfactorily simulate stand transpiration at 2-8 weeks timescale.

Another extensively used model is the Cabala model (Battaglia et al., 2004), developed by CSIRO. Cabala simulates light, nitrogen and water capture by trees and, through the use of these resources, derives estimations of tree growth (foliage, roots, and stem). Similarly to the 3-PG model, the soil is represented as a single bucket, whose size is determined by plant available water and root zone depth. Water enters the soil through rainfall and is removed by soil evaporation and transpiration (Benyon et al., 2009). The Cabala model was described and parameterized to simulate *Eucalyptus globulus* trees in Battaglia et al. (2004). In this study, the Cabala model performed reasonably well when simulating growth of younger stands.

Benyon et al. (2009) applied and compared 3PG+ and Cabala to simulate a *Eucalyptus globulus* plantation in the Green Triangle, a region located in Victoria, Australia. Both models estimated vegetation water use based on inputs of rainfall, estimated ET, simulated LAI and root depth, and soil water capacity. Simulations were in one dimension and on a daily or monthly time-step. The 3PG+ model performed better than the Cabala when simulating annual ET in plantations without access to groundwater, but both models performed poorly when groundwater was accessible to the trees. The Cabala model performed better when it came to monthly ET. In 3PG+ and Cabala, LAI is a simulated variable rather than an input variables, and it is well known that it has a strong influence on the ET. For both models, simulations of LAI constantly returned overestimated values, which affected predictions of ET. Additionally, root depth, also a simulated variable, may have affected ET values.

Process-based models enabled progress in the simulation of water use and growth by plantations. However, these models lack a more detailed representation of the transpiration process and constraints (Almeida et al., 2010; Feikema et al., 2010; Miehle et al., 2006), as was concluded by Benyon et al. (2009). The results from Benyon et al. (2009) highlight that forest growth models do not include the representation of important processes related to the movement of water within trees. For example, forest growth models do not include physiological constraints to root water uptake, which can explain how transpiration is reduced under dry conditions leading to cavitation or is regulated under well-watered conditions, such as when roots reach groundwater.

2.4.3 Tree Hydrodynamic modeling

While the Zhang curves and the forest growth models represent simpler approaches to investigate vegetation water use, they do not provide knowledge of intra-daily dynamics of stand

transpiration. A detailed representation of the transpiration process over intra-daily resolutions can identify and characterize different vegetation traits and adaptive mechanisms (Matheny et al., 2017). These mechanisms can provide, for example, important information on how trees cope with water deficit and recovery after droughts; this can in turn be critical to outline more sustainable management practices to improve tree productivity and resilience (Fatichi et al., 2016; Mencuccini et al., 2019; Verma et al., 2014).

The complex relationship between vegetation water use and environmental drivers, as discussed in Section 2.3.1, cannot be captured by simple models since it involves intricate biological and physical processes (Mencuccini et al., 2019). Transpiration is a complex process, considering that plants regulate how much water they transpire through controls at the leaf, stem, and root levels (Matheny et al., 2017). Models that can simulate the water transport below and above ground can provide important information on tree water use strategies and incorporate mechanistic representation of the internal water storage, water flow through the vegetation, xylem hydraulic properties, or stem and canopy structure (Bohrer et al., 2005; Mirfenderesgi et al., 2016).

The application of plant hydraulic models has been growing in recognition over the years for linking root water uptake, transpiration rates and carbon assimilation. Likewise, the modeling of processes such as stomatal conductance and conductivity can help to further understand the partitioning of energy fluxes between latent and sensible heat flux (Kumagai, 2001; Mirfenderesgi et al., 2018; Vrugt et al., 2001). Several quantitative approaches and applications have been developed to describe water flow in plants from the tissue to the biosphere scale. Some studies have focused on reviewing the different models and equations describing the water flow in plants, and they include an historical description (Mencuccini et al., 2019), the evolution and comparison of approaches at different spatial and temporal scales (Manzoni et al., 2013b), and a discussion regarding the relevant processes and interaction between water and plants (Fatichi et al., 2016; Matheny et al., 2017), including quantification of vegetation traits.

Most models that explicitly resolve the movement of water within the plant system rely on the cohesion-tension theory, which explains how water can be transferred upward from the soil to the atmosphere across a tree height of several meters, in the absence of osmotic pressure differences (Couvreur et al., 2018). An uninterrupted water column can extend from the roots to the leaves under tension and, as the stomata open, water is transferred to the atmosphere pulling water from the soil, through the roots and stem (Steudle, 2001). Accordingly, the system composed by the Soil, Plant, and Atmosphere is interpreted as a Continuum (SPAC) with water flowing through its different compartments following a path of decreasing water potentials (Nobel, 2009).

In this context, the first models proposed to describe transpiration fluxes used an electrical analogy, with water flowing from one compartment to the other following water potential gradients associated across plant conductive tissue with resistances to the flow (Cowan, 1965;

de Jong van Lier et al., 2008; Jones, 2009; Sperry et al., 2003; van den Honert, 1948). Recent advances in these models account for the water storage within the plant using capacitors, and link the water and CO₂ fluxes through the stomatal conductance (Bartlett et al., 2014; Cruziat et al., 2002; Daly et al., 2004a,b; Hartzell et al., 2018; Manoli et al., 2014; Manzoni et al., 2013b). Electric-circuit models commonly assume that the water flows along the SPAC occurs as a succession of steady states, whereby the water potential in the different compartments of the system adjusts instantaneously to environmental changes. Many electric-circuit models also treat the soil as a finite capacity and often consider a single compartment for each plant component (e.g., root and stem xylem) (Daly et al., 2004a; Hartzell et al., 2017). A finer resolution of resistances and capacitances might be used if a more detailed representation is desirable, but adding more layers may yield ordinary differential equations that are more difficult to solve (Chuang et al., 2006; Fatichi et al., 2016). A few electric-circuit models include formulations that account for root water compensation and other traits, although such inclusion requires the introduction of empirical parameters in the root water uptake formulation (Couvreur et al., 2012; Kennedy et al., 2019; Meunier et al., 2018).

A continuous representation of the SPAC can be achieved in models that describe the water flow in the soil and plant xylem as flow in porous media (Fruh and Kurth, 1999). Porous-media models combine the continuity equation with Darcy's law to define partial differential equations for the unsteady dynamics of the water potential across the SPAC and account for the transient response of water potential along the tree system. Some applications of these models focus on the water fluxes within the above-ground stem (Bohrer et al., 2005; Chuang et al., 2006; Kumagai, 2001), others are centred on the simulation of below-ground fluxes and the interaction between soil and roots (Amenu and Kumar, 2007; Mendel et al., 2002; Somma et al., 1998; Teodosio et al., 2017), with more recent applications looking at the whole SPAC system (Huang et al., 2017; Janott et al., 2011; Mirfenderesgi et al., 2016; Quijano and Kumar, 2015; Verma et al., 2014). Porous-media models are able to simulate a variety of processes, such as root water compensation and hydraulic redistribution (Verma et al., 2014), which are embedded in the root water uptake formulation. A canopy representation can also be accomplished by accounting for a leaf area distribution and light distribution functions throughout the stem (Christoffersen et al., 2016), and dynamic formulations for the stem capacitance and conductances can be considered (Mirfenderesgi et al., 2018).

Porous-media models that simulate the entire tree structure, with a detailed 3D representation of branches and root systems, are computationally demanding and require specific and complex parameterizations. As a result, application of these models is impracticable to simulate water flow in more than a single tree (Bohrer et al., 2005; Janott et al., 2011). One-dimensional models that lump within-tree spatial hydraulic variability in their parameters are a more practical option to represent water movement in individual trees and within stands (Amenu and Kumar, 2007; Mirfenderesgi et al., 2016, 2018; Quijano and Kumar, 2015).

Another axis of complexity that differentiates transpiration models is the level of vertical detail of the canopy representation. Single-leaf models represent the simplest approach and resolve evaporative demand from the canopy as a single surface. More advanced approaches represent the canopy as two layers, of light and shade leaves, or as multiple layers, each of a different type/size cohort of trees within the canopy (e.g., Medvigy et al., 2009). Advances in the canopy representation include the development of vertically detailed canopy representations (e.g., Bonan et al., 2018; Chen et al., 2016; Drewry et al., 2010), which led to a strong call to advance global land surface models by including a multi-layered canopy representation (Bonan et al., 2021). The complexity of the vertical representation of the canopy for the purpose of light attenuation and atmospheric demand for water could be decoupled from the complexity of the vertical representation of the hydraulic conductive pathway. For example, some models represent a vertically detailed canopy but represent the hydraulic pathway at its most simplistic form as a set of three (soil, xylem, and leaf) reservoirs (Trugman et al., 2016; Xu et al., 2016). While this approach is numerically more efficient, it may lose some of the stomatal control dynamics that are due to different rates of water storage losses at different elevations through the canopy. Specifically, it was shown that the higher leaves would experience water limitations due to storage loss sooner in the day than the lower leaves (Bohrer et al., 2005). Conversely, the continuous vertically detailed system of partial differential equations solved by porous-media models makes them a better choice to simulate plant hydraulic behavior, species-specific hydraulic traits, and their interactions with environmental drivers across different species and ecosystem types (Matheny et al., 2017), providing a more detailed representation of the tree domain and canopy structure effects than electric-circuit models or single-layer porous-media models.

Table 2.2: Key studies and application of the different modelling approaches for forest growth and water use

Reference	Application
Empirical models - Zhang curves	
Zhang et al. (1999, 2001)	These studies presented the Zhang curves, a model and tool to be used for assessing the effect of vegetation changes on catchment average water balance
Bren et al. (2006)	Derived estimates of change in water yield from grassland sites converted to <i>Radiata pine</i> by using the model of Zhang et al. (2001) to estimate the difference in water use between native forest and grassland
Brown et al. (2006)	Zhang curves were used to estimate the impact of land use change from pasture to plantation in Tasmanian catchments
Forest Growth Model - 3-PG	
Landsberg and Waring (1997)	The 3-PG model is presented as a model to simulate stand growth and biomass increment, using a monthly time step
Dye (2001)	3-PG was applied to predict growth and water use of <i>Pinus radiata</i> trees. The study highlighted the need and difficulties experienced in finding useful data sets that include descriptions of forests
Sands and Landsberg (2002)	3-PG model was parameterized for <i>E. globulus</i> trees. 3-PG provided a good simulation of future growth of blue gums stands when the model was initialised with observed biomass data at some age around or following canopy closure
Almeida et al. (2004)	3-PG model was parameterized for <i>E. grandis</i> trees. When quality data was available, 3-PG could simulate different Eucalyptus clones
Dye et al. (2004)	3-PG was applied to simulate stand growth over 12 months of stands of <i>E. grandis</i> x <i>E. camaldulensis</i> hybrid clones, representing early, mid and late rotation age
Feikema et al. (2010)	This study introduced 3-PG+, which integrated 3-PG to CAT. The integration of 3PG+ into CAT resulted in an improvement in accuracy and applicability, and provided for the spatial application of 3PG+ across diverse and mixed land use catchments
Forest Growth Model - Cabala	

Table 2.2: Key studies and application of the different modelling approaches for forest growth and water use

Reference	Application
Battaglia et al. (2004)	This study introduced the Cabala model. Cabala performed well in simulating the growth of young stands
Benyon et al. (2009)	This study applied and compared Cabala and 3PG+. The 3PG+ model performed better than the Cabala when simulating annual ET in plantations without access to groundwater, but both models performed poorly when ground-water was accessible to the trees. The Cabala model performed better when it came to monthly ET
Hydrodynamic models - Electric circuit	
Daly et al. (2004a,b)	Applied a SPAC model of soil water balance, transpiration, and photosynthesis, comparing both Leuning (1990) and Jarvis (1989) approaches for stomata behavior
Bartlett et al. (2014)	A CAM photosynthesis model was used to simulate the leaf carbon uptake and coupled to a simple SPAC approach to simulate soil water balance and different photosynthetic pathways (C3, C4, CAM)
Hartzell et al. (2017, 2018)	Model similar to Daly et al. (2004a,b), but includes a scheme for plant water storage
Hydrodynamic models - Porous media	
Kumagai (2001)	Simulated 1-D water flow through a tree stem using an experimental dataset to validate the model and parameters
Mendel et al. (2002)	Modeled root water uptake and 2-D water transport through the soil and root system as coupled processes.
Bohrer et al. (2005)	Introduced FETCH, a model that simulates water flow through a realist 1-D canopy structure, including branches.
Chuang et al. (2006)	Proposed to solve the PDE of porous media models as ODE, which could be used to derive sap flow observations into transpiration estimations
Amenu and Kumar (2007)	Modeled the root system to investigate hydraulic redistribution and root water compensation

Table 2.2: Key studies and application of the different modelling approaches for forest growth and water use

Reference	Application
Janott et al. (2011)	Combined 1D approaches to simulate water flow in the aboveground plant based on the porous media equation with root water uptake and soil water flow models also based on the porous media equation
Manoli et al. (2014)	The model coupled Richard's equation for soil moisture and plant transpiration. A 3D root water uptake model was applied to investigate overlapping root systems
Verma et al. (2014)	Simulated 1-D water flow, coupling below and above ground dynamics; solved the system of equations through a software
Mirfenderesgi et al. (2016, 2018)	Introduced FETCH2, successor of FETCH. The model simulated water flow in a 1-D vertical tree domain, including soil, roots, and stem xylem
Quijano and Kumar (2015)	Coupled below ground water transport to an ecohydrological model (MLCan) to simulate above ground dynamics

2.5 Scope of research

This project aims to understand the water use and carbon trade-off in commercial plantations, specifically focusing on quantifying and understanding the dynamics of plantation water use and carbon assimilation during the first years after plantation establishment. This work involves the collection of experimental data and the development of a tree hydrodynamic model. Figure 2.4 presents an overview of the research objectives and how they relate to each other. The research objectives are:

1: *Quantify the transpiration rates in a young *E. globulus* plantation during the first few years after its establishment.*

Measurements of actual transpiration from growing plantations over the first few years after being planted will improve the knowledge of the water cycle and provide reliable data for a more precise water balance. Water accounting models for plantation regulation, which are currently applied in South Australia and South Africa, are based only on data from mature plantations; therefore, they do not account for the dynamics of a growing plantation.

Specifically, it is necessary to understand how much water young *E. globulus* plantations use. Additionally, this data provide useful high-resolution data of tree response to different environmental conditions (e.g., heatwaves, dry conditions, and wet conditions) in different years.

2: *Analyse and quantify the relationship between water use and growth rates (i.e., Water Use Efficiency – WUE) in a growing plantation before reaching maturity.*

Afforestation with *Eucalyptus globulus* is a strong economic activity in Australia. Quantifying the variation in the amount of carbon that the trees are assimilating against the water they are using can help authorities to determine more efficient license procedures based on experimental data from growing plantations.

The WUE of a young plantation can provide information on the dynamics of carbon assimilation and water use with plantation age. The strong seasonal variability in both transpiration and carbon uptake increases the need for a more detailed and precise framework for water allocation for plantations. Taking into account the benefits of a sustainable management of *E. globulus* plantations, this aim is relevant to show the possibility for plantations to support increases in land productivity without harming the water resources available.

3: *Develop a tree hydrodynamic model to support plantation management.*

The amount of water transpired by trees can have fluctuations according to the amount of water taken up by roots, which can alter the amount of carbon fixed by trees. In this context,

the modelling of plant hydraulics can support the understanding of the water fluxes within the soil-plant-atmosphere continuum, and generate reliable projections of tree transpiration for different scenarios. In the model, this can be performed by accounting for the movement of water through the xylem, and stem and canopy structure.

This objective entails the development of the tree hydrodynamic model FETCH3, a new version of FETCH2 (Mirfenderesgi et al., 2016, 2018). FETCH3 simulates tree transpiration, coupling the trees to the soil to achieve a fully coupled soil-atmosphere-continuous model. A software package in Python will be developed and made available open-access and open source.

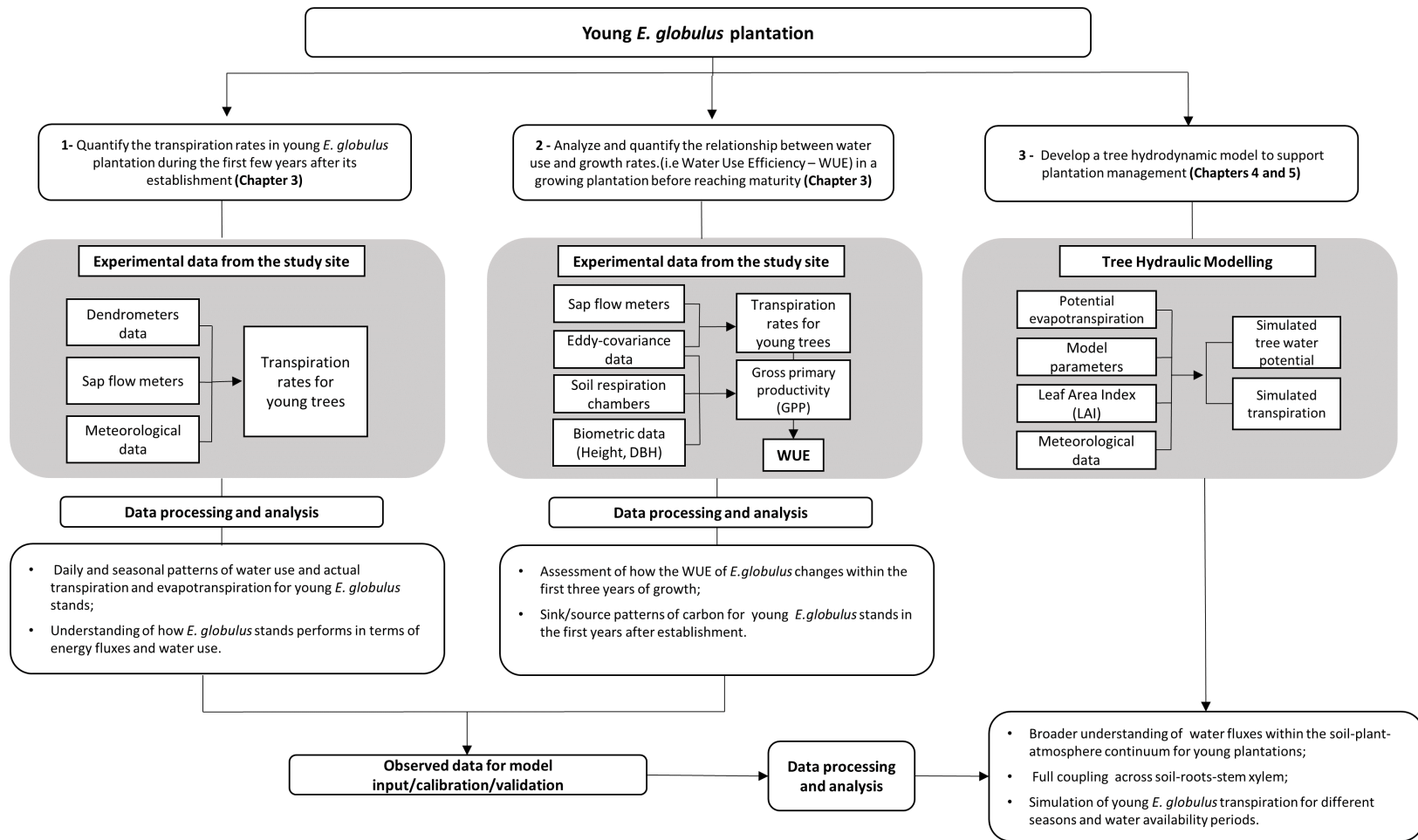


Figure 2.4: Overview of the research activities.

Chapter 3

Water and carbon fluxes in a young *Eucalyptus globulus* plantation

This chapter contains large parts of the article "Trading a little water for substantial carbon gains during the first years of a *Eucalyptus globulus* plantation" published in Agricultural and Forest Meteorology.

3.1 Aim

Determining water and carbon fluxes at the plantation scale during the first years of tree development after establishment is important to quantify plantation productivity (Baldocchi et al., 2021; Bergeron et al., 2008). The water use efficiency (WUE), which indicates how much water the trees use to grow, can provide important information for managing commercial plantations, possibly assisting land owners and government planners in allocating water for plantation activity in a sustainable manner (Pereira et al., 1986; White et al., 2016).

The aim of this study is to quantify the water and carbon fluxes in a *Eucalyptus globulus* plantation during its initial 4 years after establishment. The main objectives are (i) to quantify changes in carbon assimilation and evapotranspiration rates with stand development, and (ii) to determine the water use efficiency of a commercial plantation during the early stage of tree development. The outcome of this study provides an estimation of the trade offs between carbon and water in commercial plantations during the first years after planting.

3.2 Materials and Methods

3.2.1 Study site

The study area is located in a *E. globulus* plantation near Digby, in Southwest Victoria, Australia, within the Glenelg River Basin (Figure 3.1). The plantation was established in August 2017, with a mean tree density of approximately 1000 trees-ha⁻¹. The depth to the water table is between 5 to 10 m (Dresel et al., 2018), with trees being likely too young to reach groundwater resources (Benyon et al., 2006). Tree height at planting was between 150 mm and 300 mm, and trees were on average 11 meters tall at the end of the monitoring period (July 2021). Fertilization and weed control were applied on planting mounds before the planting, after establishment, and after 1 year to help promote growth, as it is common practice for a commercial rainfed plantation in Australia (Benyon et al., 2006).

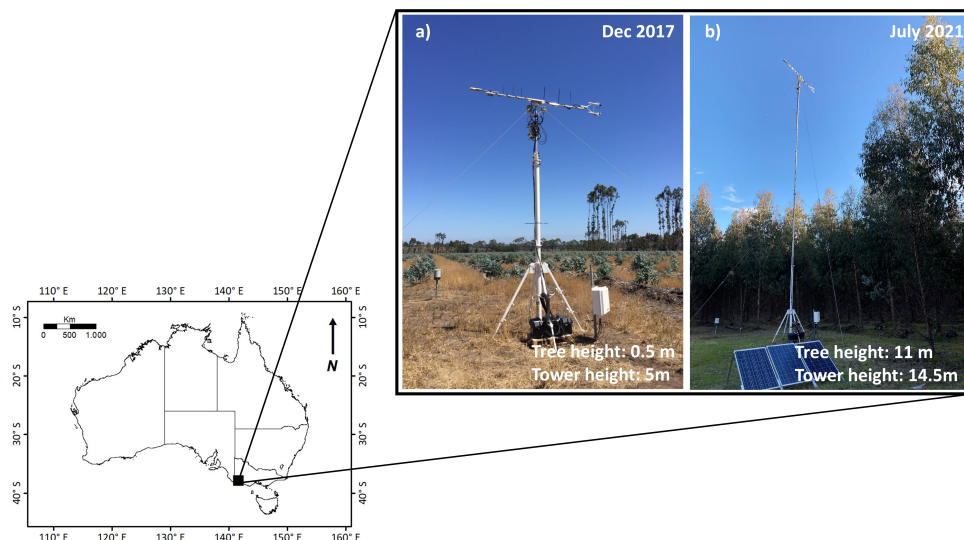


Figure 3.1: Location of the study site, and photos of the trees and the eddy covariance tower in a) December 2017, when the system was installed, and b) July 2021, at the end of the monitoring period.

The site has a long-term average annual precipitation (1950 - 2020) of 711 mm (Bureau of Meteorology station - Merino #90057, located 18 km from the site). Precipitation is dominantly in the winter (Jun - Aug) and annual precipitation in the region is highly variable. The estimated average annual potential evapotranspiration is 1020 mm (2017 - 2019) and the Koppen-Geiger climate classification is Cfb (temperate no dry season warm summer) (Dresel et al., 2018). Environmental data collected during this study (section 2.2) showed strong seasonal variation, as expected of a temperate latitude site (Figure 3.2). Daily incident solar radiation was on average approximately threefold higher in summer (34 MJ m⁻² d⁻¹) than winter (7 MJ m⁻² d⁻¹). The mean daily air temperature was 18.5 °C during the hottest month (January) and 8.9 °C

during the coldest month (July). The combination of higher rainfall and lower temperatures, hence a lower vapour pressure deficit (VPD), resulted in a generally high soil water content during this period (exceeding 40%), with low values (below 5%) observed during summer. Environmental conditions were relatively consistent across the years of the study, with 2018 being the warmest year (average of 13.42 °C - mostly due to high temperatures in the early part of the year), while daily averaged temperatures were consistent in 2019 and 2020 (12.58 °C and 12.55 °C, respectively). The annual precipitation was 749, 725 and 778 mm for 2018, 2019, and 2020, respectively (all above the long term average); however, seasonal dynamics varied, with precipitation being largest during winter in 2018 and 2019, and during the spring in 2020. Precipitation was also lower during the summer of 2018 relative to subsequent years, resulting in lower soil moisture, which reached its minimum value in February (0.02 m³m⁻³).

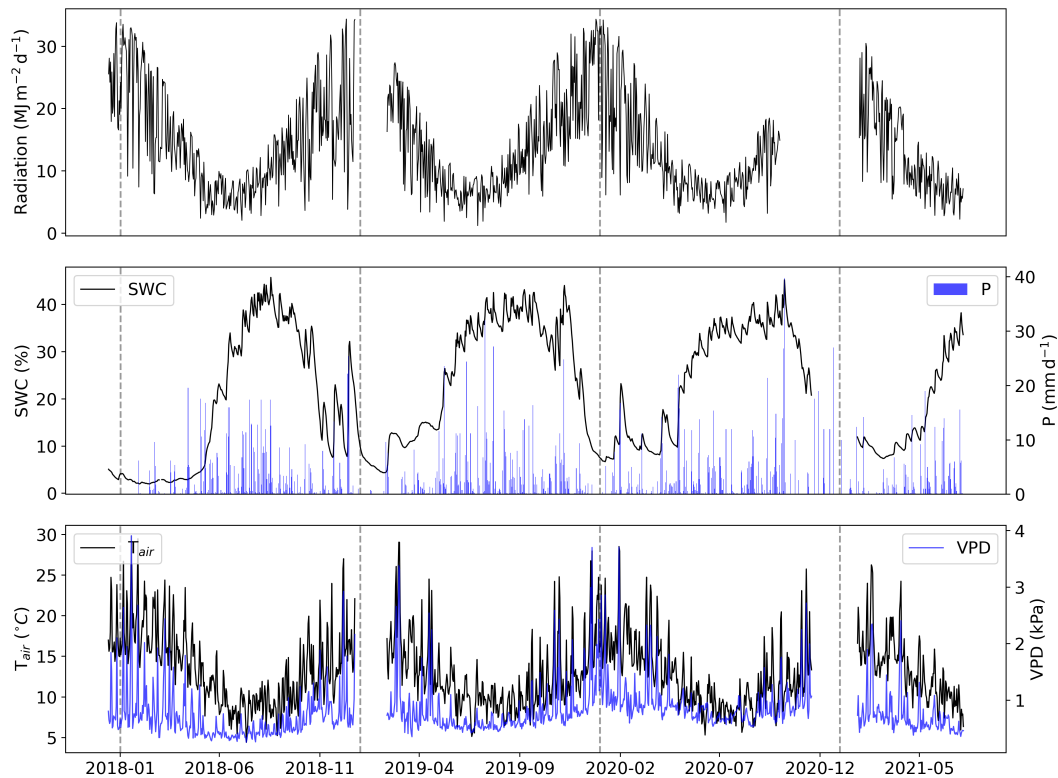


Figure 3.2: Total daily solar radiation ($\text{MJ m}^{-2} \text{d}^{-1}$) and rainfall (P , mm d^{-1}), and daily averages of the soil water content (SWC, %), air temperature (T_{air} , °C), and Vapour Pressure Deficit (VPD, kPa). Vertical dashed lines represent the transition between years.

3.2.2 Data description

Energy, water, and CO₂ fluxes were continuously measured above the tree canopy by an eddy covariance (EC) system. The EC system was installed on an extendable tower, that was raised to different heights as the trees grew. The tower height was initially 5 meters (December 2017)

and was raised to its maximum height of 14.5 meters in January 2021. Table 3.1 reports the dates when the tower was raised with the corresponding canopy heights. The sensors were positioned to maintain a distance of at least 3 m above the canopy top (Burba and Anderson, 2007). The extension of the homogeneous plantation cover over the flat surface is a guarantee for good fetch (Rodrigues et al., 2011). Increasing the tower height as the canopy developed avoids the large fetch uncertainties that would have been created if the tower had a fixed position.

Turbulent flux measurements were provided by an integrated sonic anemometer/open path infra-red gas analyser (IRGA - model IRGASON, Campbell Scientific Instruments, USA). Raw data were collected at 10 Hz frequency and accumulated to a half-hourly temporal resolution. Radiant flux measurements were provided by a four-component (incoming and outgoing short- and long-wave) radiometer (CNR4 - Kipp and Zonen, The Netherlands). The soil heat flux (G) at the soil surface was calculated using heat flux plates (model HFP01-L - Hukseflux, The Netherlands) installed at 8 cm from the soil surface and corrected using soil temperature measurements at 4 cm from the surface. The soil water content (SWC, sensors model CS650 - Campbell Scientific Instruments, USA) at 30 cm depth was measured simultaneously with the fluxes (Figure 3.2).

Additional measurements included air temperature (T_{air}) and relative humidity (RH) (HC2S3, Campbell Scientific Instruments, USA). Precipitation (P) was measured using a tipping-bucket rain gauge (CS701, Campbell Scientific Instruments, USA) installed at 1.5 m height in an open area near the tower. Rainfall measurements were cross checked and gap filled with data from the nearest Bureau of Meteorology station (Merino #90057).

The measurement period was from 14th December 2017 to 7th July 2021. There are major gaps in the data during January and part of February in 2019, and from late 2020 (starting from October for radiation and from November for the remaining variables) to late January 2021. These gaps were predominantly due to equipment failures and logistical challenges due to the COVID-19 pandemic, which interfered with the access to the site during 2020 and 2021.

Measurements of soil respiration were collected from November 2018 to November 2019 to provide an independent check on the ecosystem respiration derived from the CO₂ flux. Soil respiration was measured using a portable CO₂ gas analyser (EGM-4 - PP Systems) combined with a closed-dynamic chamber (SRC-1 - PP Systems). The measurements were collected in 9 locations within 2 plots located inside the footprint of the EC system. Both plots contained 36 trees, which were equally spaced approximately 3.5 to 4 m between rows and 2 m within rows, covering an area of approximately 250 m². Soil respiration was measured close to the tree mounds and between rows to account for the spatial variability of the fluxes within the plantation. Measurements were collected between 10 am and 1 pm, which yields a good estimate of daily averages (Almagro et al., 2009, 2013; Davidson et al., 1998; Suseela et al., 2012).

Table 3.1: Date, Age (years), average Diameter at Breast Height (DBH, mm), Tree height (m), Leaf Area Index (LAI, $\text{m}^2 \text{m}^{-2}$), and Tower height (m) during the study period. Tower height refers to the height of the EC tower after being extended.

Date	Age (years)	DBH (mm)	Height (m)	LAI ($\text{m}^2 \text{m}^{-2}$)	Tower height (m)
Dec-17	0.5		0.5		5
Sep-18	1.2	24.07	2.54	0.25	8
Nov-18	1.4	39.35	3.12	0.46	
Mar-19	1.7	48.55	4.01	0.88	
Oct-19	2.4	80.74		2.17	10
Jan-21	3.7	123.76		3.72	14.5
Jul-21	4.0	131.43	11	3.81	

Tree height and diameter at breast height (DBH) were measured to account for tree growth. From September 2018 to March 2019, tree height and DBH were manually measured in the two plots using a ruler and a measuring tape. From September 2019, DBH was measured using automatic dendrometers (DBL60 - ICT International) installed on 10 trees, and tree height was measured again in July 2021 using a clinometer. LAI was estimated from DBH and tree age using allometric equations developed by Veiga (2008) for *E. globulus* in southeast Australia (Feikema et al., 2010; Forrester et al., 2010a).

Table 3.1 reports how the DBH, tree height, and LAI increased with tree age, showing that tree growth occurred at a faster rate between September and November.

3.2.3 Data analysis

The site was equipped with a CR6 datalogger running the Easy Flux program (Campbell Scientific Inc, USA). The Easy Flux algorithm allows the logger to correct fluxes from raw high frequency data (10 Hz) into half-hourly means. It also includes the corrections commonly applied in post-processing software packages. The main corrections include detection of spikes and high frequency filtering, lag $\text{H}_2\text{O}/\text{CO}_2$ against sonic wind measurements (Foken et al., 2012), double rotation method (Lee et al., 2005), corrections for density fluctuation (WPL correction) (Webb et al., 1980), frequency response correction and sensor separation (Aubinet et al., 2012; van Dijk, 2002). Additionally, the datalogger program grades the relative quality of the fluxes following Foken et al. (2012) into categories from 1 to 9, where 1 is the best data and 9 the poorest data. Further quality assurance/quality control was applied to filter and eliminate remaining spikes and invalid data caused by heavy rainfall or system failures.

The accuracy of the dataset was assessed by calculating the energy balance closure of the site ($Q - G = LE + H$), with Q being the net radiation, G the soil heat flux, LE the latent heat flux, and H the sensible heat flux. Following Leuning et al. (2012), the energy balance was calculated considering the daily sum of fluxes (not shown) to avoid phase lags caused

by incorrect estimates of energy storage in the soil and biomass. The slope of the regression between the right- and left-hand sides of the energy balance equation was 0.82 and the R^2 was 0.94.

The Net Ecosystem Exchange (NEE) under low turbulence conditions was identified and filtered by calculating the year-specific u^* threshold for the site. The u^* threshold was calculated to filter the carbon flux measured under low turbulence conditions, and a value for each year was calculated following the change-point detection method using 1,000 iterations (Barr et al., 2013); this was applied for day- and night-time carbon fluxes following McHugh et al. (2017). NEE measurements presenting a value of u^* lower than the calculated values of 0.3 (2018) and 0.39 m s^{-1} (2019, 2020, 2021) were excluded to avoid bias in carbon flux measurements.

Gaps originated by screening and exclusion of fluxes were filled by applying a marginal distribution sampling (MDS) algorithm (Falge et al., 2001; Reichstein et al., 2005b), which considers not only the covariance between fluxes and meteorological data but also temporal auto-correlation of fluxes (Aubinet et al., 2012; Mahabbati et al., 2021). The gap filling method was performed using ReddyProc, an online tool and R package developed by the Max Planck Institute, which has been extensively used in the literature (Wutzler et al., 2018). In this method, the missing values are replaced by the average value under similar meteorological conditions.

The resulting data set was subsequently used for the partitioning of NEE into Gross Primary Productivity (GPP) and Ecosystem Respiration (ER) using the day-time based flux-partitioning algorithm introduced by Lasslop et al. (2010). In this approach, respiration is estimated from fitting a rectangular hyperbolic light–response curve. This curve is used to fit daytime NEE measurements and, as a result, respiration is estimated from the intercept of the ordinate, avoiding the use of potentially problematic nighttime data (Falge et al., 2001).

Gap filled fluxes were used to calculate annual budgets. Considering that some months were missing in the data set (January - February 2019; October/November 2020 - January 2021), the annual budgets from years with missing months were calculated using the data from previous years. Full months of missing fluxes cannot be gap filled by the most common gap filling methods; thus, this approach was used to provide reasonable estimates of yearly budgets. For January - February 2019, values from the same months in 2018 were used. For the gap in 2020, values from October or November 2019 were used. Since young trees are constantly developing and growing, the previous year fluxes were used in order to better represent the stage of tree development for that missing period.

The micrometeorological convention for fluxes is relative to the atmosphere, i.e. positive fluxes represent a gain to the atmosphere and negative fluxes a loss. The ecological convention is relative to the ecosystem, i.e. positive (negative) fluxes represents ecosystem carbon gain (loss). When presenting results regarding the fluxes between the plantation and the atmosphere, we use the micrometeorological convention. The ecological convention is used for the annual

budgets, with the terms Net Ecosystem Production (NEP), defined as $NEP = -NEE$, and Gross Ecosystem Production (GEP) defined as $GEP = -GPP$. Although NEP should also account for effects of dissolved inorganic carbon export/import (Chapin et al., 2006), we assume this to be negligible for our study.

The half-hourly gap-filled latent heat flux (LE) ($W\ m^{-2}$) was accumulated to daily time steps and converted to ET ($mm\ d^{-1} = kgH_2O\ m^{-2}d^{-1}$), and GPP was converted from $\mu molCO_2\ m^{-2}s^{-1}$ to GEP ($gC\ m^{-2}s^{-1}$), and accumulated monthly. Water Use Efficiency (WUE) was derived as $WUE = GEP/ET$ ($gC\ kg^{-1}H_2O$), using monthly accumulations of GEP and ET (Dye, 2000). Similarly, the ER/GEP monthly ratios were calculated using monthly accumulations of ER and GEP.

3.3 Results

3.3.1 Energy fluxes

The daily energy fluxes showed similar patterns during the monitored period (Figure 3.3). Sensible heat flux (H) dominated the energy partition between December and April, with the latent heat flux (LE) being larger than H during the rest of the year. In December each year, the increasing radiation and temperature favoured higher sensible heat fluxes, with a reduction in LE due to lower precipitation and soil water availability (see Figure 3.2)

The daily mean net radiation (Q) and H peaked in summer, with a daily mean maximum of 232.82, 238.03, 217.78 $W\ m^{-2}$ during 2018, 2019, and 2020, respectively, for Q, and 152.81, 150.09, 156.04 $W\ m^{-2}$, respectively, for H. Daily mean LE peaked in spring (September - November), with a maximum of 118.66, 133.62, and 129.70 $W\ m^{-2}$ during 2018 - 2020. During winter, when Q was at its minimum, H decreased considerably reaching negative values. This happened when the air temperature was higher than the soil temperature (usually with cold weather and wetter soils) creating a positive gradient of temperature from the air to the soil (Bonan, 2016).

The yearly mean Bowen ratios ($\beta = H/LE$) were 1.18, 0.88, and 0.88 for 2018, 2019, and 2020, respectively. The Bowen ratio was higher during summer and lower during winter, when it was close to zero and slightly negative in some periods. During summer, β reached a mean value of 3.04 in 2018, decreasing to 2.87 in summer 2019, and to 2.13 in summer 2020. The larger value in 2018 may reflect the physiological structure of the plantation, although as noted previously, the season was also characterised by lower rainfall and soil moisture.

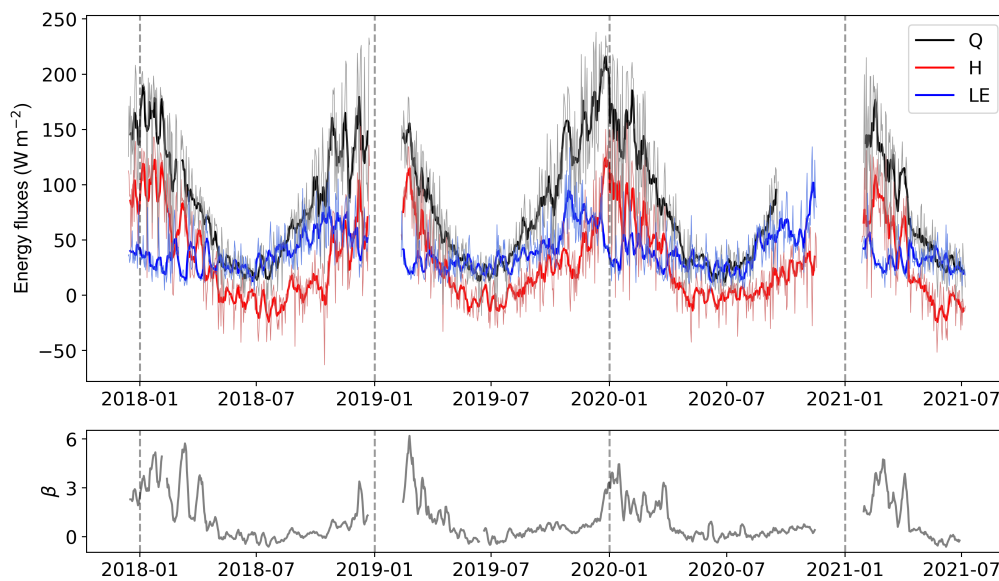


Figure 3.3: Top: daily mean net radiation (Q), sensible heat (H), and latent heat fluxes (LE) (W m^{-2}) throughout the monitored period. Bold lines represent weekly moving averages. Bottom: weekly moving averages of Bowen ratio (β). Vertical dashed lines represent transition between years.

3.3.2 Water and carbon fluxes

Mean daily ET patterns were similar between the years, with yearly mean daily values equaling about 1.50 mm in the 3 full years of measurements, with a daily maximum of 4.27, 5.1, and 5.1 mm d^{-1} for 2018, 2019, and 2020, respectively (Figure 3.4). Differences could be seen in late January and February 2020, when an increase in rainfall during the summer (32 mm in January and February 2018 against 75.4 mm for the same period in 2020) generated more ET in comparison to 2018.

Differently from ET, NEE showed a large intra- and inter-annual variability across all three monitored years. The plantation changed from behaving as a carbon source during most of 2018 and 2019 to being a carbon sink for most of 2020. The minimum daily totals of NEE were -7.41 (2018), -8.04 (2019), and -6.90 (2020) $\text{gCm}^{-2}\text{d}^{-1}$. In 2018, the ecosystem acted as a carbon source early in the year (summer and autumn), became a sink in winter and early spring, and rapidly switched to act as a source with an average NEE of 3.42 $\text{gCm}^{-2}\text{d}^{-1}$ during the last 40 days of the year. The strong seasonal cycle of NEE became less marked as trees grew in 2019 and 2020. Even though 2018 and 2019 had minimum values of NEE lower than 2020, the number of days the plantation behaved as a sink was 131 in 2018, 152 in 2019, and 250 in 2020. Taking into account the gaps in 2019 and 2020, this difference would almost certainly be

even larger.

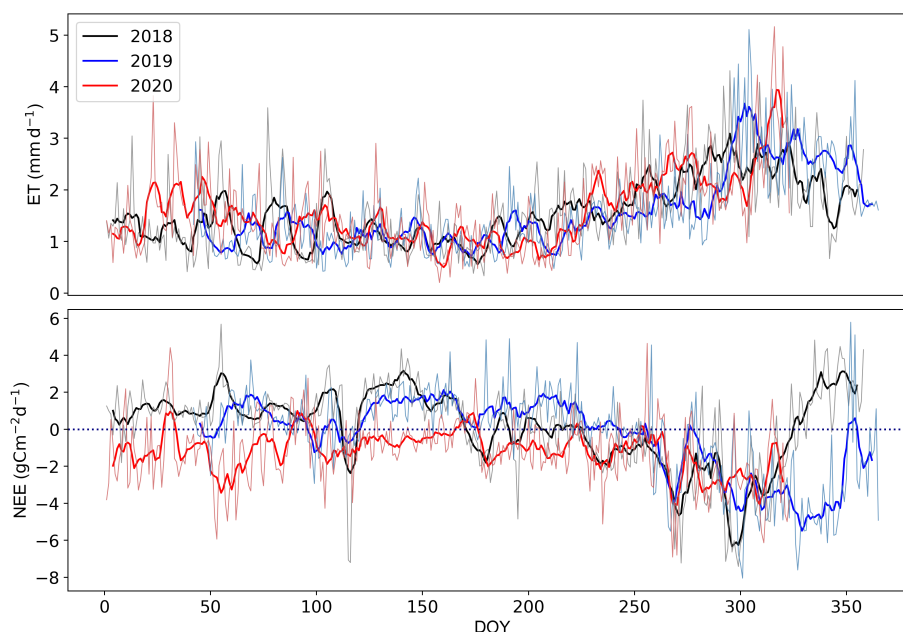


Figure 3.4: Daily total evapotranspiration (ET, mm d^{-1}) and mean daily net ecosystem exchange (NEE, $\text{gCm}^{-2}\text{d}^{-1}$) during 2018, 2019, and 2020. Thick lines represent weekly moving averages. The horizontal dashed line represents carbon neutrality.

Figure 3.5 shows the diurnal cycles of ET and NEE in different seasons during the three years from 2018 to 2020. The ET daily cycles showed similar values between years. Major differences were observed during summer, when the daily ET peak was lower in 2019 and higher in 2020. However, data are missing in January and part of February in 2019, certainly aggravating the differences between the years. ET peaks of 0.27, 0.25, and 0.22 mm h^{-1} were reached in spring in the three different years. Both maximum hourly CO_2 assimilation and ET were observed during spring, highlighting a period of high productivity for the trees.

Carbon fluxes partition

The daily accumulated GPP varied from -12.74 to -0.54 in 2018, -12.86 to -0.67 in 2019, and -9.3 to -1.21 $\text{gCm}^{-2}\text{d}^{-1}$ in 2020; the ER from 12.04 to 0.06 in 2018, 15.25 to 0.55 in 2019, and 9.52 to 0.53 $\text{gCm}^{-2}\text{d}^{-1}$ in 2020. Although the peak magnitudes were greater in 2018 and 2019, GPP and NEE showed a larger sink with stand growth, especially when comparing values registered during January and February over the years (Figure 3.6). Despite the data gap in 2020, the first part of 2021 shows that larger values of GPP are achieved in the first part of the year compared to 2018 and 2019. The modeled NEE is calculated as the sum of the modeled GPP and ER; therefore, it is not equal to the measured NEE and it is only shown in Figure 3.6 for the visualization and validation of the partition process (Lasslop et al., 2010).

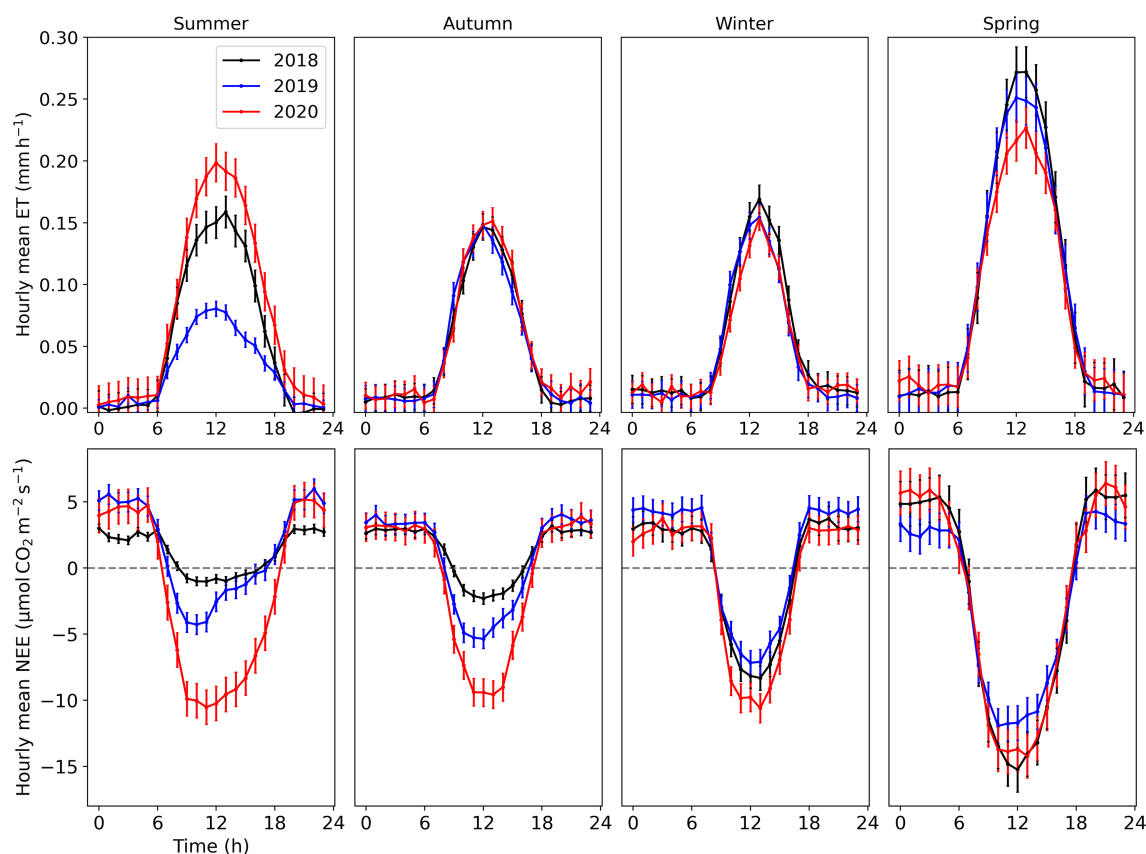


Figure 3.5: Diurnal courses (hourly means) of evapotranspiration (ET, mm h^{-1}) and net ecosystem exchange (NEE, $\mu\text{molCO}_2\text{m}^{-2}\text{s}^{-1}$) across Summer (Dec - Feb), Autumn (Mar - May), Winter (Jun - Aug), and Spring (Sep - Nov). The horizontal dashed line represents carbon neutrality. Vertical bars represent the standard error.

Soil respiration accounts for a considerable portion of ER (Law et al., 1999), and it is the largest carbon source to the atmosphere, and the second largest carbon flux after GPP (Yuste et al., 2005). Soil respiration measurements were averaged for both plots and ranged from 1.39 to 11.22 $\text{gCm}^{-2}\text{d}^{-1}$ over the measurement period. As shown in Figure 3.6, the majority of soil respiration points are smaller and close to the ER value observed for that day, thereby supporting the results of the partition of CO_2 fluxes.

Water use efficiency

After converting GPP to GEP, WUE was calculated using monthly accumulations of GEP and ET (Figure 3.7). During the monitored period, the WUE was minimum in February 2018 (1.48 $\text{gC kg}^{-1}\text{H}_2\text{O}$), and maximum in June 2020 (5.63 $\text{gC kg}^{-1}\text{H}_2\text{O}$). The yearly maximum WUE was 4.15 in 2018, 4.13 in 2019, and 5.63 $\text{gC kg}^{-1}\text{H}_2\text{O}$ in 2020. WUE increased continuously during the monitoring period following tree growth, averaging 2.86 $\text{gC kg}^{-1}\text{H}_2\text{O}$ in 2018, 3.48 $\text{gC kg}^{-1}\text{H}_2\text{O}$ in 2019, and 4.3 $\text{gC kg}^{-1}\text{H}_2\text{O}$ in 2020. Even during winter, when ET and GEP

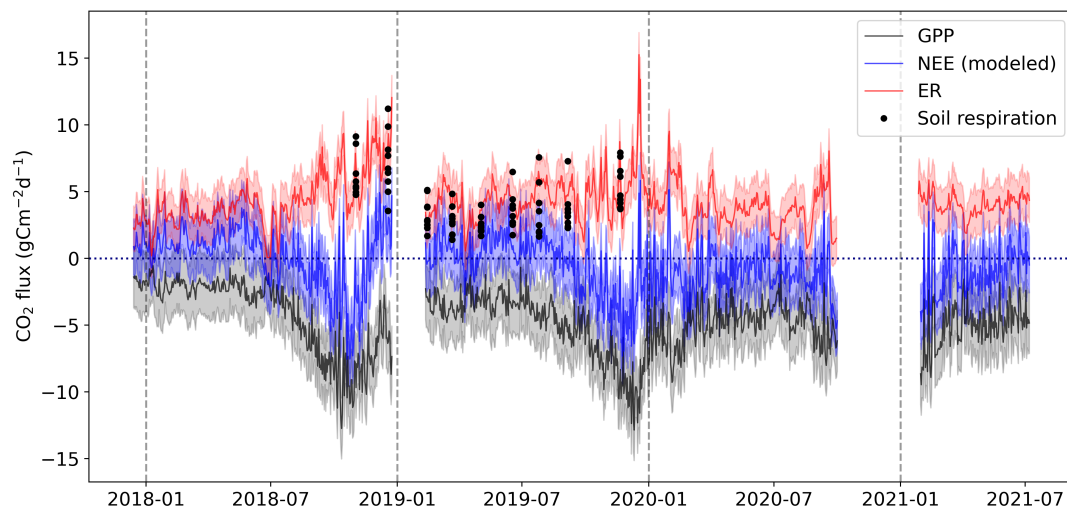


Figure 3.6: Daily accumulation of gross primary production (GPP), modeled net ecosystem exchange (NEE), and ecosystem respiration (ER) ($\text{gCm}^{-2}\text{d}^{-1}$). Shaded areas represent the standard deviation of the variables. Dots represent discrete soil respiration measurements.

were minimum, WUE increased from 3.5 in June 2018, to 3.99 in June 2019, reaching 5.63 $\text{gC kg}^{-1}\text{H}_2\text{O}$ in June 2020.

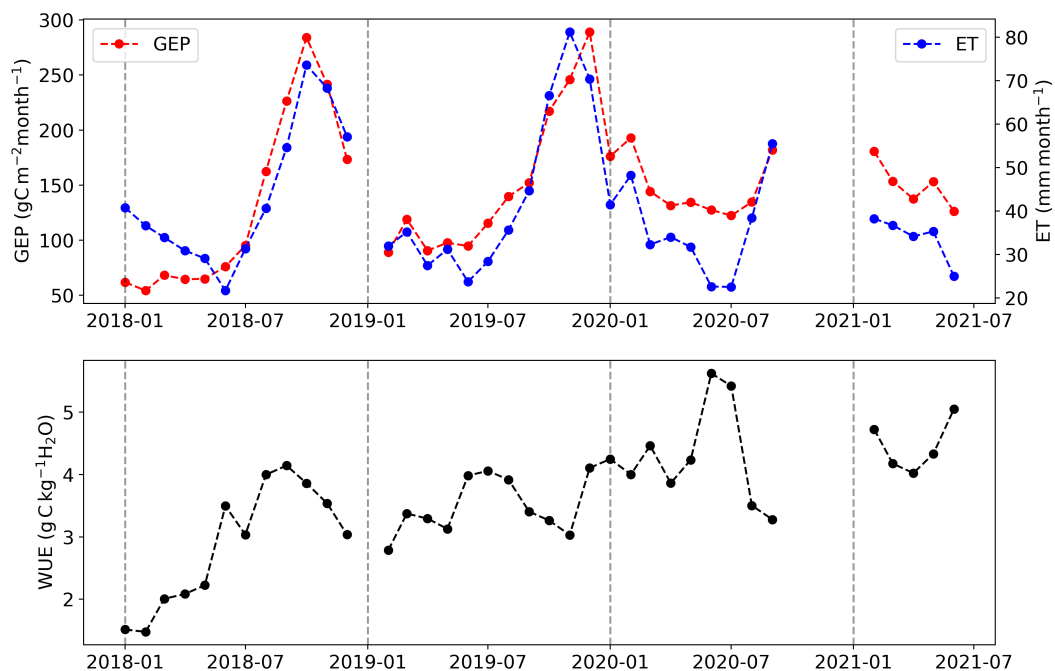


Figure 3.7: Monthly accumulation of gross ecosystem production (GEP, $\text{gC m}^{-2}\text{month}^{-1}$) and evapotranspiration (ET, mm month^{-1}), and water use efficiency (WUE) ($\text{gC kg}^{-1}\text{H}_2\text{O}$) for the study site.

Table 3.2: Annual carbon fluxes (modeled and measured NEP, GEP, and ER), ($\text{gC m}^{-2} \text{y}^{-1}$), evapotranspiration (ET, mm y^{-1}) and percentage of ET to Precipitation (P y^{-1}) for 2018, 2019, and 2020. The values are presented without estimating the missing data in incomplete months, and using the previous year to estimate missing data.

Without estimating missing months					
	NEP _{measured} ($\text{gC m}^{-2} \text{y}^{-1}$)	NEP _{modeled} ($\text{gC m}^{-2} \text{y}^{-1}$)	GEP ($\text{gC m}^{-2} \text{y}^{-1}$)	ER ($\text{gC m}^{-2} \text{y}^{-1}$)	ET (mm y^{-1})
2018	-42.54	-38.23	1538.78	1577.02	488.30
2019	131.09	132.94	1623.82	1490.87	449.92
2020	398.89	290.94	1312.52	1021.58	301.35
Estimating missing months					
2018	-54.6	-49.37	1585.04	1634.42	517.47 (70% of P)
2019	90.30	96.30	1709.50	1613.20	516.12 (71% of P)
2020	529.81	556.35	2093.61	1537.25	575.74 (74% of P)

Annual water and carbon budgets

Table 3.2 shows annual budgets with and without estimation of the missing months. The yearly ET slightly increased between 2018 and 2020, representing a 4% increase in ET/P ratios. On the other hand, the annual carbon fluxes (NEP and GEP) increased yearly with tree growth, with a shift from the ecosystem behaving as a carbon source (2018) to a carbon sink (2020) (Figure 3.8). Similarly to 2018, 2019 was a cumulative carbon source until late November when the plantation became a net sink. From 2018 to 2020, GEP increased by more than 500 gC m^{-2} . On the other hand, ER slightly decreased over the years, registering a difference of 97.17 gC m^{-2} from 2018 to 2020. Increases in GEP with respective decreases in ER resulted in a turning point for the site, when the ecosystem started to behave as a continuous sink.

An almost constant yearly ET increased the WUE throughout the study period, given the increase in growth, and hence GEP, over successive growing seasons. For example, between 2018 and 2020, annual GEP increased by 508 gC m^{-2} (32% increase from 2018), while ET varied by 58.27 mm (11% increase from 2018), which represented a change from 70% to 74% of P over this period.

3.4 Discussion

3.4.1 Water and carbon fluxes with stand age

In growing ecosystems, the combined effect of environmental variability and growth makes it challenging to determine the drivers of ET, GPP, and NEE (Chan et al., 2018; Coursolle et al., 2012; Kwon et al., 2018; Ma et al., 2019). Environmental conditions and seasonal climate patterns were mostly similar over the years of the study, suggesting that the differences in

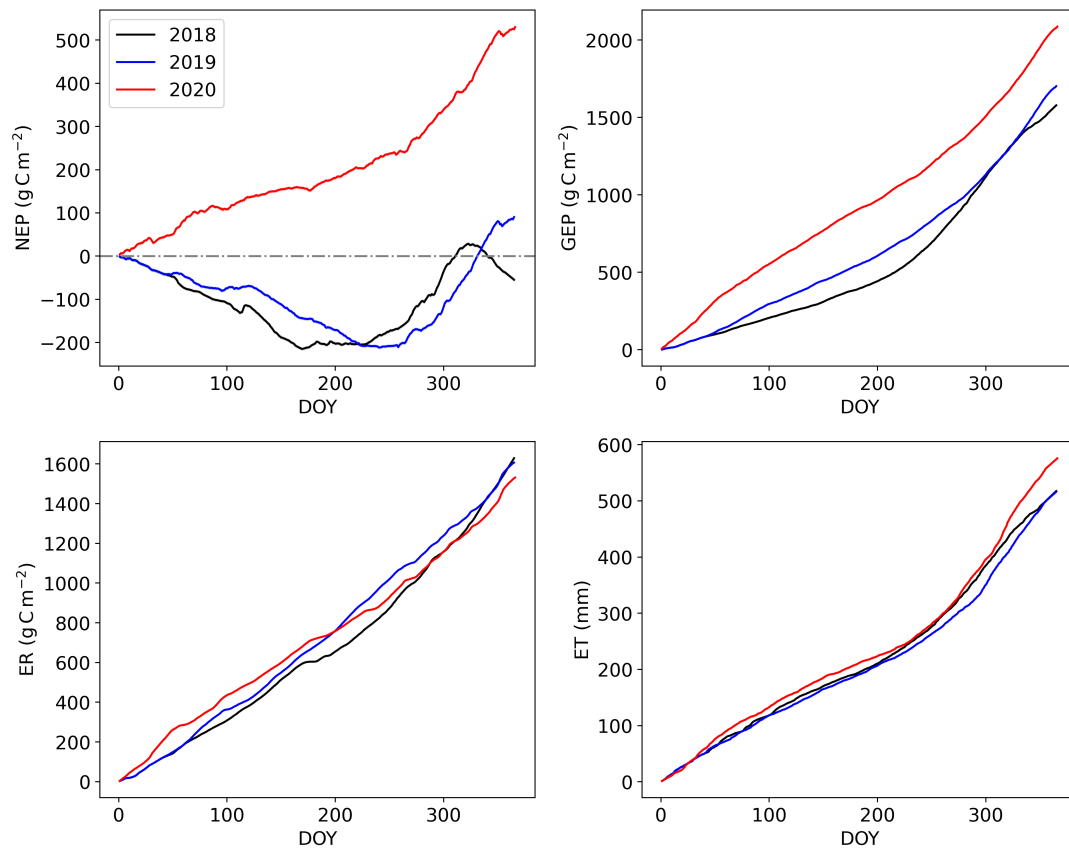


Figure 3.8: Cumulative Net Ecosystem Production (NEP, gC m^{-2}), Gross Ecosystem Production (GEP, gC m^{-2}), Ecosystem Respiration (ER, gC m^{-2}), and Evapotranspiration (ET, mm) for 2018, 2019, and 2020. The horizontal line represents carbon neutrality.

water and carbon fluxes observed during the period 2018 - 2021 can be attributed to structural changes related to tree growth, and not to the influence of meteorological variability.

As the plantation underwent structural changes between 2018 and 2021, increases in annual GEP and NEP were stronger than the increases in ET (Figure 3.8). This was likely caused by a gradual reduction in the understory weeds and grasses combined with tree LAI increases as the stand developed. LAI expansion increases shaded areas and interception, causing a decline in radiation and water for the understory vegetation (Irvine et al., 2002; Kwon et al., 2018; Vickers et al., 2012). At the study site, the understory was mostly composed of grasses, which have high transpiration rates when water and energy are available, but perish when environmental conditions become unfavorable due to higher temperatures and water stress (Pereira et al., 2007; Wiesner et al., 2019). In contrast, trees generally have more capacity to adjust transpiration, through the regulation of their stomatal conductance, which makes trees more hydrologically conservative (Jones, 2013; O'Grady et al., 1999; Pita et al., 2013).

Vegetation growth can result in transpiration increases, but the developing canopy will also offer more stomatal control over ET during drier periods than bare soil and grasses. This may have

influenced the annual ET values registered over the monitored period (Figure 3.4). Ecosystem-scale measurements of ET comprise not only tree transpiration, but also soil evaporation, understory transpiration, and canopy-intercepted water. Thus, the stages of tree development, such as changes from sparser to closer canopies, can shift the partition of ET over time, with tree transpiration increasing with tree growth as soil evaporation and understory transpiration decrease. This was observed in Ntshidi et al. (2021), where transpiration by the dense understory of young orchard stands accounted for close to 40% of the total ET. Likewise, the ET of old and young ponderosa pine plantations in Irvine et al. (2002) did not differ significantly during their study period. This was explained by the considerable transpiration by understory shrubs, which accounted for 40% of the site's LAI. For the old stands, understory vegetation was sparse and did not contribute significantly to the LAI. When studying the same ponderosa pine plantations, Law et al. (2001) identified that understory transpiration and soil evaporation were inversely proportional to the LAI, and that differences in LAI strongly influenced maximum evapotranspiration between the young and old stands.

Therefore, as the LAI increases and the canopy starts closing, a larger share of ET can switch from understory transpiration and evaporation to tree transpiration until the plantation reaches its peak (Kwon et al., 2018; Vickers et al., 2012). A similar pattern was observed for an age series of *E. globulus* trees located in Victoria (approximately 200 km from our study site), where tree transpiration and LAI increased until reaching their peak, declining afterwards (Forrester et al., 2010b). For fast-growing *E. grandis* plantations in Brazil, Almeida et al. (2007) reported a reduction in tree transpiration, LAI, and annual biomass increment when the stand age exceeded 4 years.

3.4.2 From carbon source to sink

As the plantation grows older, the assimilation of carbon in tree biomass eventually exceeds the loss from respiration and, as a consequence, NEP becomes consistently larger (Figure 3.8) (Bergeron et al., 2008; Heijmans et al., 2004; Rodrigues et al., 2011). The prevalence of GEP over ER at the site increased over time with the ER/GEP ratio decreasing from 1.03 in 2018 to 0.73 in 2020. For the global flux network, Baldocchi (2008) found an ER/GEP ratio for undisturbed ecosystems of 0.77. For Australian ecosystems, Beringer et al. (2016) estimated 0.79. Therefore, the plantation fast growing capacity allowed the site to switch to an ER/GEP ratio comparable to an undisturbed site in less than three years after establishment (Figure 3.9). Apart from June 2021, the plantation registered monthly values of $ER/GEP < 1$ starting from September 2019. This is associated with a continuously increasing NEP, which experienced a consistently increasing trend from September 2019 to the end of 2020 (Figure 3.8).

Increases in annual NEP were reported by Vickers et al. (2012) when comparing mature to young ponderosa pine stands. During their 5 year study period the NEP did not differ for mature

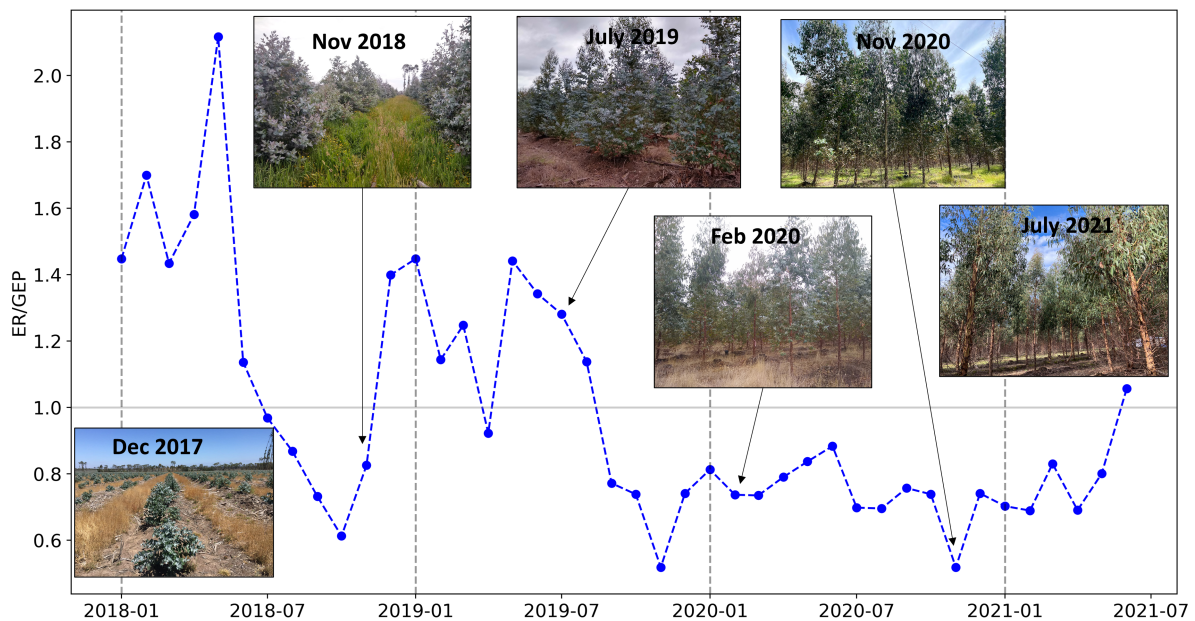


Figure 3.9: Monthly ER/GEP ratio. The horizontal line at ER/GEP=1 represents the transition between carbon source (ER/GEP > 1) and sink (ER/GEP < 1) behaviour. Vertical dashed lines represent transitions between years.

stands, whereas young stands registered a yearly increase in NEP values. The increasing NEP was associated with a 64% expansion in LAI over the 5 years. Likewise, for a young pine plantation after clear-cutting, Bracho et al. (2012) identified that carbon assimilated by developing trees was driven by LAI increases, which controlled the increments in GEP and NEP.

Only a few studies have addressed the net and gross carbon assimilated by young *Eucalyptus* plantations. Considering the particularities of each study site, it is difficult to establish a direct comparison with the results from our study. Factors such as climate, management, and age can sharply change the carbon uptake patterns of tree stands (Baldocchi et al., 2018).

For Brazilian *E. grandis* stands, which are usually managed on rotations of 6 years, the NEP increased from 993 to 1400 gC m^{-2} from the second to the third year of the management cycle (Cabral et al., 2011). Harper et al. (2014) found a mean GEP of 2720 gC m^{-2} when looking at 2 to 5 year old blue gum stands in Western Australia. Rodrigues et al. (2011) studied a Portuguese blue gum plantation before (8 to 12 year old trees) and after a felling in 2007 (1 to 3 year old trees) from 2002 to 2009. For this site, both the NEP and GEP reached their maximum value (865.56 and 2206.04 gC m^{-2} , respectively) for 8 year old trees when precipitation was also highest, and a minimum value of 11 gC m^{-2} (NEP) and 939.44 gC m^{-2} (GEP) soon after the felling. As the trees regenerated, NEP and GEP strongly increased, reaching 209.01 gC m^{-2} and 1294.05 gC m^{-2} , respectively, in 2009.

These studies show the fast-growing capacity of *Eucalyptus* stands, which influences NEP and

GEP at the ecosystem scale. Therefore, considerable increases in NEP and GEP following tree development occur for different climates and tree species. The results from the previous studies are comparable to the NEP of $556.35 \text{ gC m}^{-2}\text{y}^{-1}$ and GEP of $2093.61 \text{ gC m}^{-2}\text{y}^{-1}$ estimated in 2020 for the 3 years old trees at the study site (Table 3.2). At the study site, NEP started increasing consistently in September 2019 after about 2 years since the plantation establishment (Figure 3.8). This point can be highly variable according to differences in factors such as species, climate, understory composition, and management (Cleverly et al., 2020). For example, a Canadian pine forest became a consistent sink after 4 years (Bracho et al., 2012), and (Amiro et al., 2010) estimated a period of 10 to 20 years after a disturbance for forests across North America. Contrastingly, semi-arid ecosystems have different patterns of carbon assimilation and can behave as a source or a sink depending on wet and dry periods, which affect the carbon budget seasonally and inter-annually. This makes it difficult to estimate a period in which trees will only act as a carbon sink (Hinko-Najera et al., 2017; Tarin et al., 2020).

The present study estimated the changes in ecosystem scale carbon fluxes with stand growth. However, it is important to highlight that plantations experience other carbon inputs and losses originated from harvesting, logging, and fertilization. These components, which are part of the Net Biome Production (NBP), reflect the long-term load of CO_2 (Kutsch et al., 2010; Pregitzer and Euskirchen, 2004; Smith et al., 2008) and were not captured in this study.

3.4.3 Water use efficiency

The WUE continuously increased with stand age over the monitored period (Figure 3.7). This pattern could also be verified by other studies in growing ecosystems that investigated different species and climates (Chan et al., 2018; Irvine et al., 2004; Jassal et al., 2009; Skubel et al., 2015). For a white pine plantation in Canada (CA-TP1, Fluxnet Canada) planted in 2003, the WUE increased from 1.6 in 2003 to $4.29 \text{ gC kg}^{-1}\text{H}_2\text{O}$ at the end of the monitoring period in 2016, reaching a maximum of $5.11 \text{ gC kg}^{-1}\text{H}_2\text{O}$ in 2015 (Chan et al., 2018). Similarly, for the pine plantation described in Skubel et al. (2015), the WUE increased from 2.9 when stands were 6 years to $4.5 \text{ gC kg}^{-1}\text{H}_2\text{O}$ when they reached 11 years. In both studies, increasing productivity was a result of a larger increase in GEP than in ET, as a consequence of expanding LAI, sapwood area, and root system.

Factors such as water availability and VPD can alter how carbon is allocated in trees, favoring more stem biomass (wet periods) or root development (dry periods), thus altering the tree growth and GEP (Moroni et al., 2003; Ryan et al., 2010; Stape et al., 2004; Tfwala et al., 2019). At our study site, the WUE followed variations in the SWC. The high SWC in the first 30 cm was associated with increases in tree transpiration and carbon assimilation, since available soil water is a major factor limiting the growth in young plantations (Irvine et al., 2002; White et al.,

2016). WUE was higher when water was readily available and the ecosystem was not energy limited. During these periods, trees could transpire and assimilate CO₂ without suffering major stress or losing a great amount of water due to high temperatures.

The WUE was considerably lower during summer in 2018 (January - February). The reduced summer rainfall, and higher temperatures and VPD played important roles in this reduction, but tree development was also a crucial factor. During summer 2018, the trees were less than 1 year old; therefore, this year's summer GEP could be attributed to limited photosynthetic capacity and shallow roots, which restricted transpiration, and hence GEP, since trees could not extract water from deeper soil layers (Benyon et al., 2006; Jassal et al., 2009; Skubel et al., 2015). The sparse canopy and reduced LAI favoured more soil evaporation, which contributed to ET. Since understory grasses perish during summer, GEP contributions from the understory were minimal. In summer 2019 and 2020, the WUE consistently increased and was more than double that in 2018. For these years, a combination of higher SWC at the soil surface and increasing diameter and LAI with stand age resulted in a greater GEP and consequently higher WUE.

Few available studies investigated the variations in WUE in *Eucalyptus* stands. For mature blue gum trees (12 years) in Portugal, Pereira et al. (1986) calculated monthly variations in the WUE, registering an average of 4.2 gC kg⁻¹H₂O. Also in Portugal, Rodrigues et al. (2011) registered a maximum WUE of 4.84 gC kg⁻¹H₂O for mature trees, and 1.62 gC kg⁻¹H₂O immediately after tree felling. Two years after the felling, the WUE increased to 2.35 gC kg⁻¹H₂O. For a native *Eucalyptus* forest minimally managed since the 1970s, Griebel et al. (2020) found, from January 2013 to November 2015, an average baseline WUE of 3.02 gC kg⁻¹H₂O, with lower values during drier and hotter periods.

For our study site, the monthly averaged WUE surpassed the value of a native forest (Griebel et al., 2020) and a young commercial plantation after felling (Rodrigues et al., 2011) after approximately one year (2019) and, after that, even during summer, when the SWC reached its lowest yearly values, WUE values were above 3 gC kg⁻¹H₂O. For 2020 and 2021, most months were already in the range of those registered in mature closed-canopy blue gums (Pereira et al., 1986; Rodrigues et al., 2011).

The different responses in GEP, NEP, and WUE when comparing young and mature stands, as well as different species, climate, and treatment (i.e., natural forest and commercial plantation), highlight the need to evaluate and study stand age and species-specific characteristics. Therefore, management practices should be planned in order to maximise WUE, and thus productivity and water conservation, taking into account tree physiological dynamics and climate characteristics.

3.5 Conclusion

Fluxes of energy, water, and carbon were measured in a young *Eucalyptus globulus* plantation during the first four years after its establishment. During the study period, the NEP, GEP, and ecosystem WUE sharply increased with tree development and growth. As a result, the plantation switched from being a carbon source to a carbon sink after about 2 years, acting consistently as a sink thereafter. Tree growth and development strongly influenced the increases in NEP, GEP, and ecosystem WUE. Increases in GEP, which offset the ER resulting in a positive NEP, were caused by the expansion in LAI and, thus, photosynthesis capacity.

The results from our study show that local conditions are important in determining the water use of a plantation and that, in the early stages of growth, the increase in water consumption might be outweighed by the large gain in carbon assimilation. The water used by the plantation might, however, increase over time as the trees mature, as estimated by Dresel et al. (2018) at the same site.

The results emphasize that stands at different stages of development can show markedly different carbon fluxes and WUE. Understanding the trade-offs between water use and carbon assimilation in commercial plantations is important given the economic and ecological impacts caused by plantation establishment and expansion. Therefore, continued cultivation of large scale commercial plantations requires the application of efficient management practices.

Chapter 4

Tree hydrodynamic model development: FETCH3

This chapter contains large parts of the article and supplementary material of "Tree hydrodynamic modelling of the soil plant atmosphere continuum using FETCH3" published in Geoscientific Model Development.

4.1 Aim

The aim of this study is to present The Finite-difference Ecosystem-scale Tree Crown Hydrodynamics (FETCH3), an open source and open access tree hydrodynamic model for the simulation of the temporal and vertical dynamics of water storage and fluxes from the soil to the atmosphere, accounting for the vegetation response to environmental conditions and soil water availability. As a porous-media model, FETCH3 solves a system of three partial differential equations in a 1D domain to describe the water flow through the soil, root xylem, and stem xylem. The primary novelty of the model is a full coupling of the soil, roots, and stem xylem by clarifying the links between these 3 components of the system when re-scaling the processes into a single, continuous vertical dimension. The numerical formulation of FETCH3 was verified against exact solutions of simplified expressions of the equations, the model performance was evaluated against observational data collected during six months from a case study, and the inclusion of details of the canopy structure and stem xylem capacitance is discussed.

4.2 Model description

4.2.1 Model overview

FETCH3 builds upon FETCH2 (Mirfenderesgi et al., 2016, 2018), which is based on its precursor, the Finite Element Tree Crown Hydrodynamics (FETCH) model (Bohrer et al., 2005). FETCH simulates water flow along a tree's stem and branches accounting for the branch structure in three dimensions. Simulating the three-dimensional tree crown structure is computational demanding and can solely be applied to a single tree. As a result, FETCH2 was developed to offer a more mechanistic approach that could be scaled to entire ecosystems. To achieve this, FETCH2 simplifies branches along the vertical direction, leading to a 1D model; the equations in FETCH2 are solved using a finite difference scheme (Mirfenderesgi et al., 2016).

Similarly to FETCH and FETCH2, FETCH3 assumes that the water movement in the xylem resembles flow in porous media; as in FETCH2, a macroscopic approach is used to simulate the water fluxes across the soil, roots, and stems with the fluxes being described in one dimension along the vertical direction (Figure 4.1). As a development from FETCH2, FETCH3 presents a clearer link between the three different components of the system (i.e., soil, roots and stem), based on the conservation of water in each of the components. In its 1D domain, FETCH3 allows for the vertical variation of the soil, root xylem, and stem xylem hydraulic parameters, which are able to vary along the tree. As a result, when combined, the quantities in the equations for the roots and stem are scaled to a reference ground area, consistently with the Richardson-Richards equation for the soil. This guarantees the conservation of mass as water flows from one component to the other. The system of equations in FETCH3 is also solved differently from FETCH2. The equations in FETCH3 are discretised using the method by Celia et al. (1990) generating a system of algebraic equations combined into a single matrix, that is solved at the same time to guarantee the conservation of mass across the whole system comprising soil, roots and stem.

In FETCH3, water in a variably saturated soil is exchanged between the soil and the root system. The water flow in the soil is modelled using the Richardson-Richards equation with a term simulating the exchange of water between the soil and the roots. This term is a function of the difference in water potential between the soil and root layers; it thus results in a water sink during the day, when the water potential in the roots is low due to water loss by transpiration, but may act as a source of water to the soil during some nights, depending on the water content in different soil layers. The boundary conditions at the top and bottom of the soil column can be expressed as a flux or a value of soil water potential.

Water fluxes within roots are likewise modelled with a Richardson-Richards type equation with the same term (of the opposite sign) representing water exchange between roots and soil. Soil

and roots are coupled through this term, such that a sink of water in the soil is a source of water in the roots, and vice versa. The transfer of water between the soil and the roots is modulated by a conductance, representing the radial resistance between the bulk soil, roots surface, and root xylem, and a stress function, accounting for the reduction of the root water uptake associated with different soil moisture conditions possibly leading to water and oxygen stress. The 3D root architecture is scaled along the vertical dimension using a vertical mass distribution of the roots and an index that summarizes the extent of lateral root area per unit of ground area (Quijano and Kumar, 2015). Water fluxes through the soil are defined as the mass flow of water per unit of ground volume. Thus, when referring the water fluxes in the roots to the same water mass that was contributed by the soil, the water storage and water fluxes within the roots must be re-scaled to the ground volume and thus, when normalized by unit depth, to the ground area.

A similar approach is used to model the water flow in the above-ground xylem, which is also described with a Richardson-Richards type equation with a sink term associated with transpiration losses from the canopy to the air. This equation is commonly used to simulate water flow for a single tree (Chuang et al., 2006); however, in order to correctly couple the above-ground and the below-ground components of the system, both equations must refer the water flux to units of ground area. This ensures the water mass balance and the continuity of the fluxes from soil through the root system to the above-ground stem xylem and ultimately to the air. This conservation of flux throughout the system is important but not trivial, as the amount of roots that fits within a reference area of soil, for example, is different than the xylem area or leaf area which are located above the same area of soil. FETCH3 simulates variable plant water storage below- and above-ground by using a dynamic capacitance function that can vary in time (t) and space (z). Accounting for whole-plant water storage enables different model applications in which plant storage plays an important role, such as water use efficiency and plant hydraulic stress during dry periods (Huang et al., 2017; Li et al., 2021).

The complete system of equations simulates the water fluxes assuming a spatial distribution of trees, and their associated roots, stem xylem, and leaves, with an average cross-sectional area per unit of ground area. In this manner, FETCH3 presents a novel up-scaling technique required to properly calculate tree transpiration from small and large areas, such as a forest stand or plantations, assuming that all trees within the simulated area are similar on their dimensions and conductive parameters.

4.2.2 Governing equations

The water flow within the soil, and root and stem xylem is described as flow in porous media. Equations for the mass conservation are combined with the Darcy's equation extended to unsaturated porous media to derive an equation for the water potential in the soil, roots, and

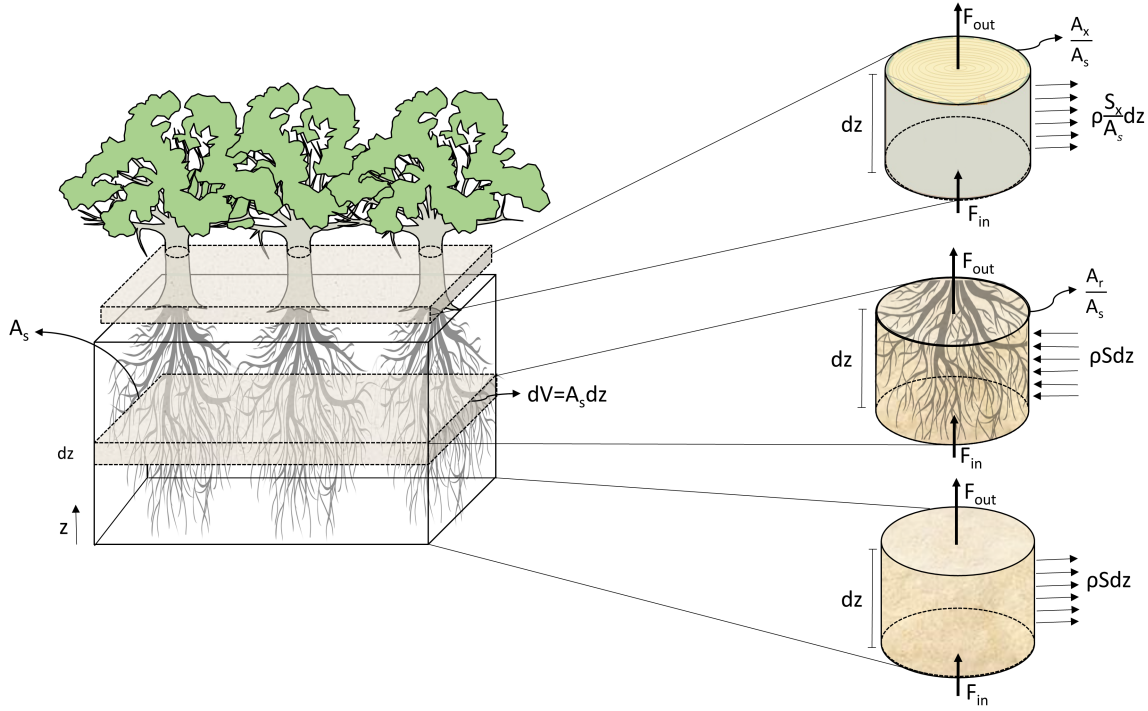


Figure 4.1: Representation of the coupling process between soil, root xylem, and stem xylem applied in the model, where A_s represents a reference ground area, dz an infinitesimal depth over an area (m), z the vertical coordinate (m), V volume of soil (m^3), ρ the density of water ($kg\ m^{-3}$), F_{in} ($kg\ s^{-1}$) the water fluxes entering and F_{out} ($kg\ s^{-1}$) exiting the volume, A_r/A_s ($m^2_{root}\ m^{-2}_{ground}$) the root xylem cross area index, A_x/A_s ($m^2_{xylem}\ m^{-2}_{ground}$) the stem xylem cross area index, S (s^{-1}) the rate at which water is extracted from the soil and enter the root xylem, and S_x ($m^2\ s^{-1}$) is the flow of water leaving the stem per unit of vertical length due to transpiration.

stem.

Soil

According to the schematic shown in Figure. 4.1 , for mass conservation, considering a volume of soil with an infinitesimal depth over an area A_s , $dV_s = A_s dz$, changes of the mass of water, M_s (kg), over time within this volume are due to the difference between the water fluxes entering, F_{in} ($kg\ s^{-1}$), and exiting, F_{out} ($kg\ s^{-1}$), the volume, and the water exchanged with the roots. This can be expressed as

$$\frac{\partial M_s}{\partial t} = F_{in} - F_{out} - \rho S dV_s, \quad (4.1)$$

where $dM_s = \rho \theta_s dV_s$, ρ is the density of water ($kg\ m^{-3}$), θ_s is the soil volumetric water content, t (s) is time, and S (s^{-1}) is the rate at which water is extracted from the soil per unit of mass of

water contained in dV_s . The term F_{out} can be written as

$$F_{out} = F_{in} + \frac{\partial F}{\partial z} dz, \quad (4.2)$$

which, substituting Eq. (4.2) into Eq. (4.1), yields

$$\rho \frac{\partial \theta_s}{\partial t} A_s dz = -\frac{\partial F}{\partial z} dz - \rho S A_s dz. \quad (4.3)$$

The flux F can be written as

$$F = \rho v_s A_s, \quad (4.4)$$

where v_s is the Darcy's velocity (m s^{-1}), expressed as

$$v_s = -K_s \left(\frac{\partial \Phi_s}{\partial z} + \rho g \right), \quad (4.5)$$

with K_s being the hydraulic conductance of the soil ($\text{m}^2 \text{s}^{-1} \text{Pa}^{-1}$), g the gravitational constant, and Φ_s the soil water potential (Pa), which in FETCH3 refers to the matric component.

Eq. (4.3) can thus be simplified into

$$C_s \frac{\partial \Phi_s}{\partial t} = \frac{d\theta_s}{d\Phi_s} \frac{\partial \Phi_s}{\partial t} = \frac{\partial}{\partial z} \left[K_s \left(\frac{\partial \Phi_s}{\partial z} + \rho g \right) \right] - S. \quad (4.6)$$

where $C_s = \frac{\partial \theta}{\partial \Phi_s}$ (Pa^{-1}) is the soil water capacitance, and z (m) is distance along vertical direction, assuming positive represents upward flux. The relationships between K_s , Φ_s and θ_s are modelled according to van Genuchten (1980) (refer to Section 4.5).

Roots

Following the same procedure as the soil, the conservation of water mass in the roots, with $dM_r = \rho \theta_r A_r dz$, results in

$$\rho \frac{\partial (\theta_r A_r)}{\partial t} dz = \rho \frac{\partial}{\partial z} \left[K_r A_r \left(\frac{\partial \Phi_r}{\partial z} + \rho g \right) \right] dz + \rho S A_s dz. \quad (4.7)$$

Dividing Eq. (4.7) by $\rho A_s dz$ leads to

$$C_r \frac{\partial \Phi_r}{\partial t} = \frac{d}{d\Phi_r} \left(\frac{\theta_r A_r}{A_s} \right) \frac{\partial \Phi_r}{\partial t} = \frac{\partial}{\partial z} \left[K_r \frac{A_r}{A_s} \left(\frac{\partial \Phi_r}{\partial z} + \rho g \right) \right] + S, \quad (4.8)$$

where C_r (Pa^{-1}) is the root xylem water capacitance, Φ_r (Pa) is the root water potential, θ_r is

the root volumetric water content, K_r ($\text{m}^2 \text{s}^{-1} \text{Pa}^{-1}$) is the effective axial hydraulic conductivity of the roots, and A_r/A_s ($\text{m}_{root}^2 \text{m}_{ground}^{-2}$) is the root cross sectional area index, representing the total root cross-sectional area at a given elevation per unit of ground area.

Stem

The conservation of water mass in the stems, with $dM_x = \rho\theta_x A_x dz$, results in

$$\rho \frac{\partial(\theta_x A_x)}{\partial t} dz = \rho \frac{\partial}{\partial z} \left[K_x A_x \left(\frac{\partial \Phi_x}{\partial z} + \rho g \right) \right] dz - \rho S_x dz, \quad (4.9)$$

where Φ_x (Pa) is the stem xylem water potential, K_x ($\text{m}^2 \text{s}^{-1} \text{Pa}^{-1}$) is the effective axial hydraulic conductivity of the stem xylem, and S_x ($\text{m}^2 \text{s}^{-1}$) is the flow of water leaving the stem per unit of vertical length due to transpiration. It is convenient to express S_x as a function of transpiration per unit of ground area, T (m s^{-1}), which is most commonly measured. Because transpiration along the stem depends on the leaf area, S_x can be expressed as $l A_s T$, with $l(z)$ ($\text{m}^2 \text{m}^{-2} \text{m}^{-1}$) being the leaf area per ground area per unit of stem height, and A_s the ground area.

Dividing Eq. (4.9) by $\rho A_s dz$, such that water fluxes across soil, roots, and stem are expressed in terms of ground area, one obtains

$$C_x \frac{\partial \Phi_x}{\partial t} = \frac{d}{d\Phi_x} \left(\frac{\theta_x A_x}{A_s} \right) \frac{\partial \Phi_x}{\partial t} = \frac{\partial}{\partial z} \left[K_x \frac{A_x}{A_s} \left(\frac{\partial \Phi_x}{\partial z} + \rho g \right) \right] - \frac{S_x}{A_s}, \quad (4.10)$$

where C_x (Pa^{-1}) is the stem xylem water capacitance, θ_x ($\text{m}^3 \text{m}^{-3}$) is the stem xylem volumetric water content, and A_x/A_s ($\text{m}_{stem}^2 \text{m}_{ground}^{-2}$) is the stem xylem cross-sectional area index. This index can be calculated from the tree sapwood area and stand density (typically reported for forest plots as number of trees per hectare), representing the total sapwood area per unit of ground area. The cross sectional area indices applied to the roots and stem xylem guarantee the conservation of water as it flows across soil, roots, and stem.

4.2.3 Root water uptake and transpiration

Eqs. (4.6) and (4.8) are coupled through the exchange of water between the soil and roots. The term S is modelled as a function of the difference between the water potential in the soil and the roots. This approach, introduced by Gardner (1960), was applied in several studies (Amenu and Kumar, 2007; Herkelrath et al., 1977; Mendel et al., 2002). Accordingly, S (s^{-1}) is expressed as

$$S(z, t) = k_{s,rad} f(\theta_s(z, t)) \cdot \frac{A_{ls}}{A_s}(z) \cdot \frac{r(z)}{\int_{z_{r_i}}^{z_{r_j}} r(z) dz} \cdot (\Phi_s(z, t) - \Phi_r(z, t)), \quad (4.11)$$

where $k_{s,rad}$ ($\text{m}^3\text{s}^{-1}\text{m}_{root}^{-2}\text{Pa}^{-1}$) is the soil-to-root radial conductance per unit of root surface area, $f(\theta_s)$ is a dimensionless reduction function due to soil moisture, $r(z)$ the root mass distribution, with z_{r_i} and z_{r_j} (m) representing the elevation of the bottom and top of the roots, and A_{ls}/A_s ($\text{m}_{root}^2\text{m}_{ground}^{-2}$) is an index defining the lateral root surface area per unit of ground, representing the root surface area taking up water from the soil. The vertical profile of root mass distribution represents the percentage of roots contained in different soil layer. The product of these two terms in Eq. 4.11 provides the portion of roots contributing to the exchange of water between soil and roots; this changes with depth depending on how the roots are vertically distributed.

The water lost to the atmosphere is calculated using a transpiration function that depends on meteorological variables and limits the amount of water leaving the stomata as a function of the stem water potential. FETCH3 allows for the implementation of different transpiration functions, and a complete description of the transpiration formulation applied in this study is in Section 4.4. Accordingly, S_x/A_s (s^{-1}) reads

$$\frac{S_x}{A_s}(z, t) = T \cdot l(z), \quad (4.12)$$

where T (m s^{-1}) is the transpiration rate defined per unit of ground area, which is distributed along the canopy height via the leaf area density distribution ($l(z)$, $\text{m}^2 \text{m}^{-2} \text{m}^{-1}$), which is the leaf area per unit of ground area per unit of height, which integrates vertically to the leaf area index (LAI). This effectively assumes that transpiration is proportional to leaf area throughout the depth of the canopy. We have found that in canopies where most leaves are concentrated near the upper layers, the results are not very sensitive to this simplification. More complex representations of the vertical distribution of transpiration through the canopy depth have been developed. Such vertically detailed canopy transpiration models assume, for example, that transpiration is vertically distributed proportionally to vertical light extinction through the depth of the canopy (Bohrer et al., 2009; Shaw and Schumann, 1992), or that transpiration rate is vertically distributed as a function that combines light attenuation and the vertical profiles of other physical radiative forcing, such as turbulence, wind speed, temperature, and humidity (Bonan et al., 2018; Drewry et al., 2010). Such transpiration models can be easily implemented in FETCH3 by replacing Eq. (4.12) with a more elaborate vertical redistribution scheme, provided that the vertical descriptions of the required parameters for leaf area density, light attenuation and other physical forcing are available for the simulated forest plot.

4.3 Numerical scheme

The water flow across the soil-plant-atmosphere continuum is lumped along the vertical direction. The domain of the model can be idealized as the combination of the vertical extent of the soil and the tree (root and stem) xylem, with exchange of water between the soil and the roots (Figure 4.2).

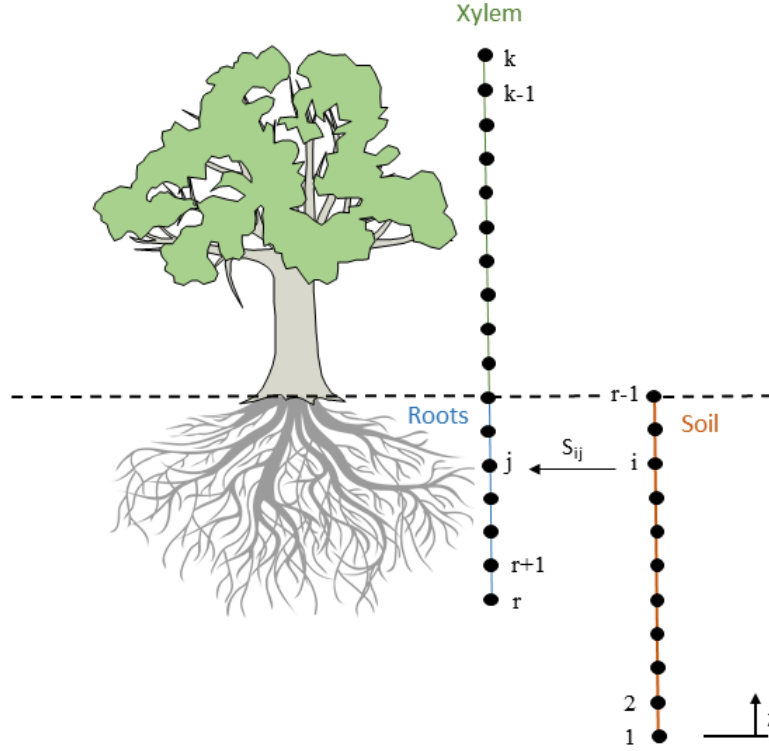


Figure 4.2: Representation of the model domain

Each of Eqs. (4.6), (4.8), and (4.10) can be written as

$$C \frac{\partial \Phi}{\partial t} = - \frac{\partial F}{\partial z} \pm S^*, \quad (4.13)$$

where C is a capacitance, Φ is the water potential, F is the flux, and S^* is a source or sink term accounting for either the exchange of water between soil and roots or the water loss due to transpiration for the stem xylem.

Eq. (4.13) is discretized using constant intervals, Δz , with values of Φ calculated at the nodes and fluxes, F , calculated between nodes. Eq. (4.13) is approximated using a fully implicit backward Euler method, and its discretized form for a generic node i reads

$$C_i^{n+1} \frac{\Phi_i^{n+1} - \Phi_i^n}{\Delta t} = - \frac{F_{i+1/2}^{n+1} - F_{i-1/2}^{n+1}}{\Delta z} \pm S_i^{*,n+1}, \quad (4.14)$$

where n and $n+1$ indicate values of the variables at two consecutive times, with $\Delta t = t^{n+1} - t^n$. The fluxes can be then expressed as

$$F_{i+1/2}^{n+1} = -K_{i+1/2}^{n+1} \frac{\Phi_{i+1}^{n+1} - \Phi_i^{n+1}}{\Delta z} - K_{i+1/2}^{n+1} \rho g \quad (4.15)$$

$$F_{i-1/2}^{n+1} = -K_{i-1/2}^{n+1} \frac{\Phi_i^{n+1} - \Phi_{i-1}^{n+1}}{\Delta z} - K_{i-1/2}^{n+1} \rho g, \quad (4.16)$$

where K is the hydraulic conductance (including the ratio of the areas appearing in Eqs. 4.8 and 4.10).

In the following, a full detailed description of the numerical approximation of the system of equations and the implementation of initial and boundary conditions are presented.

4.3.1 Discretization

Eqs. (4.6), (4.8), and (4.10) are approximated as in Eq. (4.13), and are then combined and solved at the same time with the standard fully implicit Picard method following the scheme in Celia et al. (1990).

With m denoting the number of the Picard iteration, and the subscript i denoting a generic node, Eq. (4.14) reads

$$C_i^{n+1,m} \frac{(\Phi_i^{n+1,m+1} - \Phi_i^n)}{\Delta t} = +K_{i+1/2}^{n+1,m} \frac{(\Phi_{i+1}^{n+1,m+1} - \Phi_i^{n+1,m+1})}{(\Delta z)^2} - K_{i-1/2}^{n+1,m} \frac{(\Phi_i^{n+1,m+1} - \Phi_{i-1}^{n+1,m+1})}{(\Delta z)^2} + \frac{K_{i+1/2}^{n+1,m}}{\Delta z} \rho g - \frac{K_{i-1/2}^{n+1,m}}{\Delta z} \rho g \pm S_i^{*,n+1}, \quad (4.17)$$

with the hydraulic conductance calculated in the middle of two neighbouring nodes as

$$K_{i-1/2}^{n+1,m} = \frac{1}{2}(K_{i-1}^{n+1,m} + K_i^{n+1,m}) \quad (4.18)$$

$$K_{i+1/2}^{n+1,m} = \frac{1}{2}(K_i^{n+1,m} + K_{i+1}^{n+1,m}). \quad (4.19)$$

The terms in Eq. (4.17) can be rearranged as

$$\begin{aligned}
 & \frac{C_i^{n+1,m}}{\Delta t} (\Phi_i^{n+1,m+1} - \Phi_i^{n+1,m}) + \frac{C_i^{n+1,m}}{\Delta t} (\Phi_i^{n+1,m} - \Phi_i^n) = + \frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} (\Phi_{i+1}^{n+1,m+1} - \Phi_{i+1}^{n+1,m}) \\
 & + \frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} (\Phi_{i+1}^{n+1,m}) - \frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} (\Phi_i^{n+1,m+1} - \Phi_i^{n+1,m}) - \frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} (\Phi_i^{n+1,m}) + \frac{K_{i+1/2}^{n+1,m}}{\Delta z} \rho g \\
 & - \frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} (\Phi_i^{n+1,m+1} - \Phi_i^{n+1,m}) - \frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} (\Phi_i^{n+1,m}) + \frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} (\Phi_{i-1}^{n+1,m+1} - \Phi_{i-1}^{n+1,m}) \\
 & + \frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} (\Phi_{i-1}^{n+1,m}) - \frac{K_{i-1/2}^{n+1,m}}{\Delta z} \rho g \pm S_i^{*,n+1}, \quad (4.20)
 \end{aligned}$$

which, defining the increment $\delta\Phi^{n+1,m} = \Phi^{n+1,m+1} - \Phi^{n+1,m}$, yields

$$\begin{aligned}
 & \frac{C_i^{n+1,m}}{\Delta t} (\delta\Phi_i^{n+1,m}) + \frac{C_i^{n+1,m}}{\Delta t} (\Phi_i^{n+1,m} - \Phi_i^n) = + \frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} (\delta\Phi_{i+1}^{n+1,m}) + \frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} (\Phi_{i+1}^{n+1,m}) \\
 & - \frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} (\delta\Phi_i^{n+1,m}) - \frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} (\Phi_i^{n+1,m}) + \frac{K_{i+1/2}^{n+1,m}}{\Delta z} \rho g - \frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} (\delta\Phi_i^{n+1,m}) \\
 & - \frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} (\Phi_i^{n+1,m}) + \frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} (\delta\Phi_{i-1}^{n+1,m}) + \frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} (\Phi_{i-1}^{n+1,m}) - \frac{K_{i-1/2}^{n+1,m}}{\Delta z} \rho g \pm S_i^{*,n+1}. \quad (4.21)
 \end{aligned}$$

Reorganizing Eq.(4.21), one obtains

$$\begin{aligned}
 & \left(\frac{-K_{i-1/2}^{n+1,m}}{\Delta z^2} \right) \delta\Phi_{i-1}^{n+1,m} + \left(\frac{C_i^{n+1,m}}{\Delta t} + \frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} + \frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} \right) \delta\Phi_i^{n+1,m} + \left(\frac{-K_{i+1/2}^{n+1,m}}{\Delta z^2} \right) \delta\Phi_{i+1}^{n+1,m} = \\
 & \frac{1}{\Delta z^2} \left[K_{i+1/2}^{n+1,m} (\Phi_{i+1}^{n+1,m} - \Phi_i^{n+1,m}) - K_{i-1/2}^{n+1,m} (\Phi_i^{n+1,m} - \Phi_{i-1}^{n+1,m}) \right] + \frac{K_{i+1/2}^{n+1,m}}{\Delta z} \rho g - \frac{K_{i-1/2}^{n+1,m}}{\Delta z} \rho g \\
 & - \frac{C_i^{n+1,m}}{\Delta t} (\Phi_i^{n+1,m} - \Phi_i^n) \pm S_i^{*,n+1}. \quad (4.22)
 \end{aligned}$$

For the soil, $S_i^{*,n+1}$ is a sink of water (i.e., the sign '-' applies to Eq. (4.22))

$$S_i^{*,n+1} = k_{e,rad_i}(z, t) \cdot f(\theta_i^{n+1,m+1})(\Phi_{s_i}^{n+1,m+1} - \Phi_{r_j}^{n+1,m+1}), \quad (4.23)$$

where the subscripts s and r refer to soil and roots, and j is a node of the roots corresponding to the same elevation z as i for the soil (Figure 4.2). k_{e,rad_i} represents the effective radial conductance.

Introducing the increments $\delta\Phi^{n+1,m}$ for the water potentials, the expression for $S_i^{*,n+1}$ in the soil

(with the sign '-' in Eq. 4.21) and root xylem (with the sign '+' in Eq. 4.21) is

$$S_i^{*,n+1}(z, t) = k_{e,rad_i} f(\theta_i^{n+1,m+1}) (\delta \Phi_{s_i}^{n+1,m} - \delta \Phi_{r_j}^{n+1,m} - \Phi_{s_i}^{n+1,m} + \Phi_{r_j}^{n+1,m}). \quad (4.24)$$

Reorganizing the equation in the same form of Eq. (4.22), and substituting the expression for the sink term (Eq. 4.24), the numerical approximation for the soil nodes becomes:

$$\begin{aligned} & -\frac{K_{s_i-1/2}^{n+1,m}}{\Delta z^2} \delta \Phi_{s_i-1}^{n+1,m} + \left[\frac{C_{s_i}^{n+1,m}}{\Delta t} + \frac{K_{s_i+1/2}^{n+1,m}}{\Delta z^2} + \frac{K_{s_i-1/2}^{n+1,m}}{\Delta z^2} + k_{e,rad_i} f(\theta_i^{n+1,m+1}) \right] \delta \Phi_{s_i}^{n+1,m} \\ & - \frac{K_{s_i+1/2}^{n+1,m}}{\Delta z^2} \delta \Phi_{s_i+1}^{n+1,m} - k_{e,rad_i} f(\theta_i^{n+1,m+1}) \delta \Phi_{r_j} = \frac{1}{\Delta z^2} \left[K_{s_i+1/2}^{n+1,m} (\Phi_{s_i+1}^{n+1,m} - \Phi_{s_i}^{n+1,m}) \right. \\ & \quad \left. - K_{s_i-1/2}^{n+1,m} (\Phi_{s_i}^{n+1,m} - \Phi_{s_i-1}^{n+1,m}) \right] + \frac{K_{s_i+1/2}^{n+1,m}}{\Delta z} \rho g - \frac{K_{s_i-1/2}^{n+1,m}}{\Delta z} \rho g \\ & \quad - \frac{C_{s_i}^{n+1,m}}{\Delta t} (\Phi_{s_i}^{n+1,m} - \Phi_{s_i}^n) - k_{e,rad_i} f(\theta_i^{n+1,m+1}) (\Phi_{s_i}^{n+1,m} - \Phi_{r_j}^{n+1,m}). \quad (4.25) \end{aligned}$$

Likewise, the numerical approximation for the nodes of the root xylem becomes

$$\begin{aligned} & -\frac{K_{r_i-1/2}^{n+1,m}}{\Delta z^2} \delta \Phi_{r_i-1}^{n+1,m} + \left[\frac{C_{r_i}^{n+1,m}}{\Delta t} + \frac{K_{r_i+1/2}^{n+1,m}}{\Delta z^2} + \frac{K_{r_i-1/2}^{n+1,m}}{\Delta z^2} + k_{e,rad_i} f(\theta_i^{n+1,m+1}) \right] \delta \Phi_{r_i}^{n+1,m} \\ & - \frac{K_{r_i+1/2}^{n+1,m}}{\Delta z^2} \delta \Phi_{r_i+1}^{n+1,m} - k_{e,rad_i} f(\theta_i^{n+1,m+1}) \delta \Phi_{s_j} = \frac{1}{\Delta z^2} \left[K_{r_i+1/2}^{n+1,m} (\Phi_{r_i+1}^{n+1,m} - \Phi_{r_i}^{n+1,m}) \right. \\ & \quad \left. - K_{r_i-1/2}^{n+1,m} (\Phi_{r_i}^{n+1,m} - \Phi_{r_i-1}^{n+1,m}) \right] + \frac{K_{r_i+1/2}^{n+1,m}}{\Delta z} \rho g - \frac{K_{r_i-1/2}^{n+1,m}}{\Delta z} \rho g \\ & \quad - \frac{C_{r_i}^{n+1,m}}{\Delta t} (\Phi_{r_i}^{n+1,m} - \Phi_{r_i}^n) + k_{e,rad_i} f(\theta_i^{n+1,m+1}) (\Phi_{s_i}^{n+1,m} - \Phi_{r_j}^{n+1,m}). \quad (4.26) \end{aligned}$$

A similar approximation can be written for the stem xylem, where the sink term is simpler than for the soil and root xylem, because it does not include interactions between nodes at different elevations.

Considering, for example, that both soil and roots have the same depth (i.e, roots are present from the bottom to the top of the soil column), the system of partial differential equations can be approximated by a system of algebraic equations for each iteration within each time step. In matrix format, this system of equations can be written as

$$\begin{pmatrix}
 b_1 & c_1 & 0 & 0 & \dots & K_{rad,1} & 0 & 0 & \dots \\
 a_2 & b_2 & c_2 & 0 & \dots & 0 & K_{rad,2} & 0 & \dots \\
 0 & a_3 & b_3 & c_3 & \dots & 0 & 0 & K_{rad,3} & \dots \\
 \dots & & & & & & & & \\
 K_{rad,1} & 0 & \dots & & & 0 & b_r & c_r & 0 & \dots \\
 0 & K_{rad,2} & 0 & \dots & & 0 & a_{r+1} & b_{r+1} & c_{r+1} & 0 & \dots \\
 0 & 0 & K_{rad,3} & 0 & \dots & 0 & 0 & a_{r+2} & b_{r+2} & c_{r+2} & 0 & \dots \\
 \dots & & & & & & & & & & \\
 \dots & & & & & & & & & & \dots & a_{k-2} & b_{k-2} & c_{k-2} & 0 \\
 \dots & & & & & & & & & & \dots & 0 & a_{k-1} & b_{k-1} & c_{k-1} \\
 \dots & & & & & & & & & & \dots & 0 & 0 & a_k & b_k
 \end{pmatrix} \cdot \begin{pmatrix} \delta_1^{n+1,m} \\ \delta_2^{n+1,m} \\ \delta_3^{n+1,m} \\ \dots \\ \delta_r^{n+1,m} \\ \delta_{r+1}^{n+1,m} \\ \delta_{r+2}^{n+1,m} \\ \dots \\ \delta_{k-2}^{n+1,m} \\ \delta_{k-1}^{n+1,m} \\ \delta_k^{n+1,m} \end{pmatrix} = \begin{pmatrix} d_1^{n+1} \\ d_2^{n+1} \\ d_3^{n+1} \\ \dots \\ d_r^{n+1} \\ d_{r+1}^{n+1} \\ d_{r+2}^{n+1} \\ \dots \\ d_{k-2}^{n+1} \\ d_{k-1}^{n+1} \\ d_k^{n+1} \end{pmatrix},$$

where the subscripts r and k denote the bottom of the roots and top of the canopy, respectively, and the node 1 represents the bottom of the soil (Figure 4.2). The system of algebraic equations is solved to find the values of $\delta\Phi_i^{n+1}$; this is then added to $\Phi_i^{n,m}$ to calculate $\Phi_i^{n+1,m+1}$, which is then used to calculate the new values of the coefficients for the calculation of a new value of $\delta\Phi_i$. These iterations proceed until the difference of two successive calculated water potentials in each node approaches a predefined tolerance, δ , such that

$$|\Phi^{n+1,m+1} - \Phi^{n+1,m}| \leq \delta. \quad (4.27)$$

The matrix coefficients for a generic node within the soil read

$$a_i = -\frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} \quad (4.28)$$

$$b_i = \left(\frac{C_i^{n+1,m}}{\Delta t} + \frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} + \frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} + k_{e,rad_i} f(\theta_i^{n+1,m+1}) \right) \quad (4.29)$$

$$c_i = -\frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} \quad (4.30)$$

$$K_{rad,i} = -k_{e,rad_i} f(\theta_i^{n+1,m+1}) \quad (4.31)$$

$$d_i = \frac{1}{\Delta z^2} \left[K_{i+1/2}^{n+1,m} (\Phi_{i+1}^{n+1,m} - \Phi_i^{n+1,m}) - K_{i-1/2}^{n+1,m} (\Phi_i^{n+1,m} - \Phi_{i-1}^{n+1,m}) \right] \quad (4.32)$$

$$+ \rho g \frac{(K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m})}{\Delta z} - \frac{C_i^{n+1,m}}{\Delta t} (\Phi_i^{n+1,m} - \Phi_i^n) - k_{e,rad_i} f(\theta_i^{n+1,m+1}) (\Phi_{s_i}^{n+1,m} - \Phi_{r_j}^{n+1,m}). \quad (4.33)$$

The coefficients for a generic node associated with the roots are

$$a_i = -\frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} \quad (4.34)$$

$$b_i = \left(\frac{C_i^{n+1,m}}{\Delta t} + \frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} + \frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} + k_{e,rad_i} f(\theta_i^{n+1,m+1}) \right) \quad (4.35)$$

$$c_i = -\frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} \quad (4.36)$$

$$K_{rad,i} = -k_{e,rad_i} f(\theta_i^{n+1,m+1}) \quad (4.37)$$

$$d_i = \frac{1}{\Delta z^2} \left[K_{i+1/2}^{n+1,m} (\Phi_{i+1}^{n+1,m} - \Phi_i^{n+1,m}) - K_{i-1/2}^{n+1,m} (\Phi_i^{n+1,m} - \Phi_{i-1}^{n+1,m}) \right] \quad (4.38)$$

$$+ \rho g \frac{(K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m})}{\Delta z} - \frac{C_i^{n+1,m}}{\Delta t} (\Phi_i^{n+1,m} - \Phi_i^n) + k_{e,rad_i} f(\theta_i^{n+1,m+1}) (\Phi_{s_i}^{n+1,m} - \Phi_{r_j}^{n+1,m}). \quad (4.39)$$

The coefficients for a generic node of the stem read

$$a_i = -\frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} \quad (4.40)$$

$$b_i = \left(\frac{C_i^{n+1,m}}{\Delta t} + \frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} + \frac{K_{i-1/2}^{n+1,m}}{\Delta z^2} \right) \quad (4.41)$$

$$c_i = -\frac{K_{i+1/2}^{n+1,m}}{\Delta z^2} \quad (4.42)$$

$$d_i = \frac{1}{\Delta z^2} \left[K_{i+1/2}^{n+1,m} (\Phi_{i+1}^{n+1,m} - \Phi_i^{n+1,m}) - K_{i-1/2}^{n+1,m} (\Phi_i^{n+1,m} - \Phi_{i-1}^{n+1,m}) \right] \quad (4.43)$$

$$+ \rho g \frac{(K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m})}{\Delta z} - \frac{C_i^{n+1,m}}{\Delta t} (\Phi_i^{n+1,m} - \Phi_i^n) - S_{x,i}^{n+1}/A_{s,i}, \quad (4.44)$$

with details on the expression of S_x provided in Section 4.4.

4.3.2 Initial and boundary conditions

The initial condition needs to be a known function $\Phi_0 = \Phi(z, 0)$ across the soil, roots and stem. A common choice is to assume that soil and both root and stem xylem are in hydrostatic conditions (i.e., $\Phi_0 = -\rho g z$), without water fluxes occurring across the system.

Boundary conditions are required at the bottom of the roots, at the top of the stem, and at the bottom and top of the soil. No-flux boundary conditions are the default conditions for the bottom of the roots and top of the stem. No flux boundary conditions can be imposed at the bottom of the soil and a specific flux can be imposed at the top of the soil as infiltration. Conditions at the

bottom of the soil can be also provided as a given value of water potential or as free drainage.

No flux boundary conditions can be specified by imposing the flux at the corresponding nodes to be zero. For example, in the case of the bottom of the soil, for $i = 1$, a no flux condition is obtained by imposing $F_{1-1/2}^{n+1} = 0$ in Eq. (4.14).

Accordingly, the terms in the matrix summarizing the system of equation for node 1 are

$$\begin{aligned}
 b_1 &= \frac{C_1^{n+1,m}}{\Delta t} + \frac{K_{1+1/2}^{n+1,m}}{\Delta z^2} + k_{e,rad_1} f(\theta_i^{n+1,m+1}), \\
 c_1 &= -\frac{K_{1+1/2}^{n+1,m}}{\Delta z^2}, \\
 K_{rad,1} &= -k_{e,rad_1} f(\theta_i^{n+1,m+1}) \\
 d_1 &= \frac{1}{\Delta z^2} \left[K_{1+1/2}^{n+1,m} (\Phi_2^{n+1,m} - \Phi_1^{n+1,m}) \right] + \rho g \frac{K_{1+1/2}^{n+1,m}}{\Delta z} \\
 &\quad - \frac{C_1^{n+1,m}}{\Delta t} (\Phi_1^{n+1,m} - \Phi_1^n) - k_{e,rad_1} f(\theta_i^{n+1,m+1}) (\Phi_1^{n+1,m} - \Phi_{r_j}^{n+1,m}).
 \end{aligned}$$

The conditions at the bottom of the roots and top of the stem can be obtained in a similar way.

In the case of a specified water potential boundary condition (Dirichlet), the potential at the bottom of the soil is a series of known values, such that $\phi(1, t) = \Phi_{b_i}$. This leads to the following expression for $\Phi_2^{n+1,m+1}$:

$$\begin{aligned}
 &\left(\frac{-K_{2-1/2}^{n+1,m}}{\Delta z^2} \right) \delta \Phi_{b_i} + \left(\frac{C_2^{n+1,m}}{\Delta t} + \frac{K_{2+1/2}^{n+1,m}}{\Delta z^2} + \frac{K_{2-1/2}^{n+1,m}}{\Delta z^2} + k_{e,rad_2} f(\theta_2^{n+1,m+1}) \right) \delta \Phi_2^{n+1,m} + \\
 &\quad \left(\frac{-K_{2+1/2}^{n+1,m}}{\Delta z^2} \right) \delta \Phi_3^{n+1,m} - k_{e,rad_2} f(\theta_2^{n+1,m+1}) \delta \Phi_{s_i} = \\
 &\quad \frac{1}{\Delta z^2} \left[K_{2+1/2}^{n+1,m} (\Phi_3^{n+1,m} - \Phi_2^{n+1,m}) - K_{2-1/2}^{n+1,m} (\Phi_2^{n+1,m} - \Phi_{b_i}^{n+1,m}) \right] + \frac{K_{2+1/2}^{n+1,m}}{\Delta z} \rho g \\
 &\quad - \frac{K_{2-1/2}^{n+1,m}}{\Delta z} \rho g - \frac{C_2^{n+1,m}}{\Delta t} (\Phi_2^{n+1,m} - \Phi_2^n) - k_{e,rad_2} f(\theta_2^{n+1,m+1}) (\Phi_{s_i}^{n+1,m} - \Phi_{r_j}^{n+1,m}) \quad (4.45)
 \end{aligned}$$

Reorganizing in the form of the matrix yields

$$a_2 = \frac{-(K_{2-1/2}^{n+1,m})}{\Delta z^2} \quad (4.46)$$

$$b_2 = \left(\frac{C_2^{n+1,m}}{\Delta t} + \frac{K_{2+1/2}^{n+1,m}}{\Delta z^2} + \frac{K_{2-1/2}^{n+1,m}}{\Delta z^2} + k_{e,rad_2} f(\theta_2^{n+1,m+1}) \right) \quad (4.47)$$

$$c_2 = \frac{-(K_{2+1/2}^{n+1,m})}{\Delta z^2} \quad (4.48)$$

$$K_{rad,2} = -k_{e,rad_2} f(\theta_2^{n+1,m+1}) \quad (4.49)$$

$$d_2 = \frac{1}{\Delta z^2} \left[K_{2+1/2}^{n+1,m} (\Phi_3^{n+1,m} - \Phi_2^{n+1,m}) - K_{2-1/2}^{n+1,m} (\Phi_2^{n+1,m} - \Phi_{b_i}^{n+1,m}) \right] \quad (4.50)$$

$$+ \rho g \frac{(K_{2+1/2}^{n+1,m} - K_{2-1/2}^{n+1,m})}{\Delta z} - \frac{C_2^{n+1,m}}{\Delta t} (\Phi_2^{n+1,m} - \Phi_2^n) - k_{e,rad_2} f(\theta_2^{n+1,m+1}) (\Phi_{s_i}^{n+1,m} - \Phi_{r_j}^{n+1,m}) \quad (4.51)$$

In the case of soil profile with deep groundwater levels, the water flux at the bottom of the soil is only due to gravity; therefore, the pressure gradient is equal to zero:

$$F_{1-1/2}^{n+1} = -K_{1-1/2}^{n+1} (0 + \rho g), \quad (4.52)$$

$$C_1^{n+1} \frac{\Phi_1^{n+1} - \Phi_1^n}{\Delta t} = -\frac{F_{1+1/2}^{n+1} - (-K_{1-1/2}^{n+1} \rho g)}{\Delta z} - S(\Phi_1^n). \quad (4.53)$$

Reorganizing in matrix format, one obtains

$$b_1 = \frac{C_1^{n+1,m}}{\Delta t} + \frac{K_{1+1/2}^{n+1,m}}{\Delta z^2} + k_{e,rad_1} f(\theta_1^{n+1,m+1}),$$

$$c_1 = -\frac{K_{1+1/2}^{n+1,m}}{\Delta z^2},$$

$$K_{rad,1} = -k_{e,rad_1} f(\theta_1^{n+1,m+1})$$

$$d_1 = \frac{1}{\Delta z^2} \left[K_{1+1/2}^{n+1,m} (\Phi_2^{n+1,m} - \Phi_1^{n+1,m}) \right] + \rho g \frac{K_{1+1/2}^{n+1,m}}{\Delta z} - \frac{C_1^{n+1,m}}{\Delta t} (\Phi_1^{n+1,m} - \Phi_1^n) \\ - \frac{K_{1-1/2}^{n+1,m} \rho g}{\Delta z} - k_{e,rad_1} f(\theta_1^{n+1,m+1}) (\Phi_1^{n+1,m} - \Phi_{r_j}^{n+1,m}).$$

For the top of the soil column, considering inputs from infiltration, the flux at the node $i = s$ is known as $F_{s+1/2}^{n+1} = q_{inf}$, resulting in

$$C_s \frac{\Phi_s^{n+1} - \Phi_s^n}{\Delta t} = -\frac{q_{inf} - F_{s-1/2}^{n+1}}{\Delta z} - S, \quad (4.54)$$

$$q_{inf}^{n+1,m+1} = \max \left(-q, -(\theta_{sat} - \theta_s^{n+1,m+1}) \cdot \left(\frac{\Delta z}{\Delta t} \right) \right), \quad (4.55)$$

where q is the precipitation rate.

Reorganizing in matrix format leads to

$$\begin{aligned} a_s &= -\frac{K_{s-1/2}^{n+1,m}}{\Delta z^2}, \\ b_s &= \frac{C_s^{n+1,m}}{\Delta t} + \frac{K_{s-1/2}^{n+1,m}}{\Delta z^2} + k_{e,rad_s} f(\theta_s^{n+1,m+1}), \\ K_{rad_s} &= -k_{e,rad_s} f(\theta_s^{n+1,m+1}), \\ d_s &= \frac{1}{\Delta z^2} \left[-K_{s-1/2}^{n+1,m} (\Phi_s^{n+1,m} - \Phi_{s-1}^{n+1,m}) \right] - \rho g \frac{K_{s-1/2}^{n+1,m}}{\Delta z} - \frac{C_s^{n+1,m}}{\Delta t} (\Phi_s^{n+1,m} - \Phi_s^n) \\ &\quad - k_{e,rad_s} f(\theta_s^{n+1,m+1}) (\Phi_s^{n+1,m} - \Phi_{r_j}^{n+1,m}) + \frac{q_{inf}}{\Delta z}. \end{aligned}$$

4.4 Penman-Monteith transpiration

Transpiration is calculated in a subroutine and can thus be defined according to the formulation assigned by the user. Here, we present how transpiration was calculated in Section 4.2.3, following the formulation implemented in (Verma et al., 2014).

The water that the trees lose to the atmosphere via transpiration S_x/A_s is calculated as

$$\frac{S_x}{A_s} = T \cdot l(z), \quad (4.56)$$

where T is the transpiration rate per unit of ground area (m s^{-1}). Transpiration is distributed throughout the canopy height using the leaf area density (LAD) ($l(z)$, $\text{m}^2 \text{ m}^{-2} \text{ m}^{-1}$), which is the leaf area index (LAI) distributed along the canopy height z .

Transpiration is calculated through the Penman-Monteith formulation (Allen et al., 1998; Verma et al., 2014):

$$T = \left[\frac{Q_n \Delta + C_p D g_a}{\lambda [\Delta g_c + \gamma (g_c + g_a)]} \right] g_c, \quad (4.57)$$

where Q_n (W m^{-2}) is the net radiation, Δ ($\text{kg m}^{-1} \text{s}^{-2} \text{K}^{-1}$) is the slope of the saturation vapor

pressure curve for a given temperature, C_p ($\text{kg m}^{-1}\text{s}^{-2}\text{K}^{-1}$) is the specific heat of air, D is the vapour pressure deficit (VPD) (Pa), λ ($\text{kg m}^{-1}\text{s}^{-2}$) is the latent heat of vaporisation, g_a (m s^{-1}) is the aerodynamic conductance, γ ($\text{kg m s}^{-2}\text{K}^{-1}$) is the psychrometric constant, and g_c (m s^{-1}) is the canopy conductance. In this study, Q_n is assumed to be 60% of incoming solar radiation; this is different from Verma et al. (2014), where this term was calculated as 70% of solar radiation. Δ is calculated as

$$\Delta = \left[\frac{4098}{(T_a - 35.85)^2} \right] e_{sat}, \quad (4.58)$$

where e_{sat} (Pa) is the saturation vapour pressure for a given temperature of the atmosphere (T_a), given as

$$e_{sat} = 611 \exp \left[\frac{17.27(T_a - 273.15)}{T_a - 35.85} \right]. \quad (4.59)$$

The canopy conductance, g_c , is calculated as

$$g_c = \left[\frac{g_s g_b}{g_s + g_b} \right] LAI, \quad (4.60)$$

where LAI is the leaf area index, g_b (m s^{-1}) is the leaf boundary layer conductance per m^2 of leaf area and g_s (m s^{-1}) is the stomatal conductance, which depends on both plant physiology and environmental factors. In the present model, g_s is modeled as (Jarvis, 1976),

$$g_s = g_{smax} \cdot f(S_{in}) \cdot f(T_a) \cdot f(D) \cdot f(\Phi_x), \quad (4.61)$$

where g_{smax} (m s^{-1}) is the maximum stomatal conductance, and $f(S_{in})$, $f(T_a)$, $f(D)$, and $f(\Phi_x)$ are empirical functions [-], representing the behavior of g_s according to variations in solar radiation, temperature, VPD, and leaf water potential, respectively. These functions vary between 0 and 1, and are calculated as

$$f(S_{in}) = 1 - \exp(-k_r S_{in}), \quad (4.62)$$

$$f(T_a) = 1 - k_t (T_a - T_{opt})^2, \quad (4.63)$$

$$f(D) = \frac{1}{(1 + D k_d)}, \quad (4.64)$$

$$f(\Phi_x) = \left[1 + \left(\frac{\Phi_{xleaf}}{\Phi_{x50}} \right)^{n_l} \right]^{-1}, \quad (4.65)$$

where k_r , k_t , k_d and n_l are empirical constants, T_{opt} is the air temperature at which $f(T_a)$ is 1, and Φ_{x50} is the leaf water potential at 50% loss of conductivity. $f(\Phi_x)$ represents the inverse polynomial expression commonly used to express the effect of water potential on xylem conductance (Manzoni et al., 2013a).

Since nighttime transpiration is not always zero under low or absent solar radiation (ie., during heat waves), a different approach was used to model night time transpiration, as in

$$E_n = E_{max} \cdot f(T_a) \cdot f(D) \cdot f(\Phi_x), \quad (4.66)$$

where E_{max} (m s^{-1}) is the maximum night time transpiration, which was estimated in Verma et al. (2014).

4.5 Soil water retention relationships

The relationships between K_s , Φ_s and θ_s are modeled according to van Genuchten (1980) as

$$K_s = \frac{k_{s,sat}}{\rho g} \Theta^{1/2} \left[1 - (1 - \Theta^{1/n})^m \right]^2, \quad (4.67)$$

$$C_s = \frac{d\theta_s}{d\Phi_s} = \frac{d\theta_s}{\rho g dh_s} = \frac{-\alpha m (\theta_{sat} - \theta_{res})}{\rho g (1 - m)} \Theta^{1/m} (1 - \Theta^{1/m})^m, \quad (4.68)$$

where,

$$\Theta(z, t) = \frac{\theta - \theta_{res}}{\theta_{sat} - \theta_{res}}, \quad (4.69)$$

$$\theta = \theta_{res} + \frac{(\theta_{sat} - \theta_{res})}{[1 + (\alpha|h|)^n]^m}, \quad (4.70)$$

$$m = 1 - \frac{1}{n}, \quad (4.71)$$

$$0 < m < 1, \quad (4.72)$$

where K_s ($\text{m}^2 \text{s}^{-1} \text{Pa}^{-1}$) is the effective soil hydraulic conductivity, $k_{s,sat}$ (m s^{-1}) is the soil hydraulic conductivity under saturated soil conditions, θ_{sat} and θ_{res} indicate the saturated and residual values of the soil volumetric water content, and C_s (Pa^{-1}) is the soil capacitance.

4.6 Hydraulic conductances

4.6.1 Root radial conductance

The exchange of water between soil and roots depends of the amount of roots contained in different soil layers. The fraction of roots at different soil depths is modeled following Vrugt et al. (2001), with the function

$$r(z) = \left(1 - \frac{z}{z_{r_j} - z_{r_i}}\right) \exp\left(\frac{-qz}{z_{r_j} - z_{r_i}}\right) \quad z_{r_i} \leq z \leq z_{r_j}, \quad (4.73)$$

where z is the vertical coordinate (positive upwards), z_{r_j} is the elevation of the top of the roots, and z_{r_i} is the elevation of the bottom of the roots, with $z_{r_j} - z_{r_i}$ the root depth.

Using Eq.(4.73), the root water uptake is written as

$$S(z, t) = k_{s,rad} f(\theta_s(z, t)) \cdot \frac{A_{ls}}{A_s}(z) \cdot \frac{r(z)}{\int_{z_{r_i}}^{z_{r_j}} r(z) dz} \cdot (\Phi_s(z, t) - \Phi_r(z, t)), \quad (4.74)$$

where $f(\theta)$ [-] is a water stress reduction function, Φ_s , and Φ_r , are water potentials (Pa) for the soil and roots, respectively, $k_{s,rad}$ ($\text{m}^3\text{s}^{-1}\text{m}_{\text{root}}^{-2}\text{Pa}^{-1}$) is the soil-to-root radial conductance per unit of root surface area, and A_{ls}/A_s ($\text{m}_{\text{root}}^2\text{m}_{\text{ground}}^{-2}$) is an index defining the lateral root surface area per unit of ground, representing the root surface area taking up water from the soil. The $f(\theta)$ function is written as,

$$f(\theta) = \begin{cases} 0 & \theta \leq \theta_1, \\ \frac{(\theta - \theta_1)}{(\theta_2 - \theta_1)} & \theta_1 < \theta \leq \theta_2, \\ 1 & \theta > \theta_2, \end{cases} \quad (4.75)$$

$$(4.76)$$

$$(4.77)$$

where θ_1 and θ_2 are the soil water content below which root water uptake is ceased and the soil water content below which root water uptake start decreasing, respectively (Feddes et al., 1976). The current version of FETCH3 does not consider water stress by low oxygen conditions (anoxia).

4.6.2 Axial conductances

The effective axial conductance of the roots, K_r ($\text{m}^2\text{s}^{-1}\text{Pa}^{-1}$), can be defined as

$$K_r = \frac{k_r}{\rho g} \frac{A_r}{A_s}, \quad (4.78)$$

with,

$$k_r(z, t) = k_{sax} \cdot \left(1 - \frac{1}{1 + \exp(a_p(\Phi_r - b_p))}\right), \quad (4.79)$$

where k_{sax} (m s^{-1}) is the specific axial conductivity for the root system, and a_p (Pa^{-1}) and b_p (Pa) are parameters for the root xylem cavitation curve, which describes the vulnerability of xylem to cavitation.

The effective hydraulic conductance of the axial stem xylem, K_x ($\text{m}^2 \text{s}^{-1} \text{Pa}^{-1}$), is defined similarly as Eq. (4.78), as

$$K_x = \frac{k_x}{\rho g} \frac{A_x}{A_s}, \quad (4.80)$$

with

$$k_x(\Phi_x(z, t)) = k_{max} \cdot \left(1 - \frac{1}{1 + \exp(a_p(\Phi_x - b_p))} \right), \quad (4.81)$$

where k_{max} (m s^{-1}) is the maximum conductivity of saturated stem xylem, and a_p (Pa^{-1}) and b_p (Pa) are the shape parameters of the cavitation curve.

Chapter 5

FETCH3 model applications

This chapter contains large parts of the article "Tree hydrodynamic modelling of the soil plant atmosphere continuum using FETCH3" published in Geoscientific Model Development.

5.1 Aim

Three applications were used to i) test the correctness of the numerical scheme against analytical solutions, ii) compare results to a published case study, iii) show the implementation of a leaf area density profile and a xylem capacitance function dependent on the xylem water potential, and iv) calibrate the model against measured sap flow data. Figure 5.1 summarizes the model applications described in this chapter.

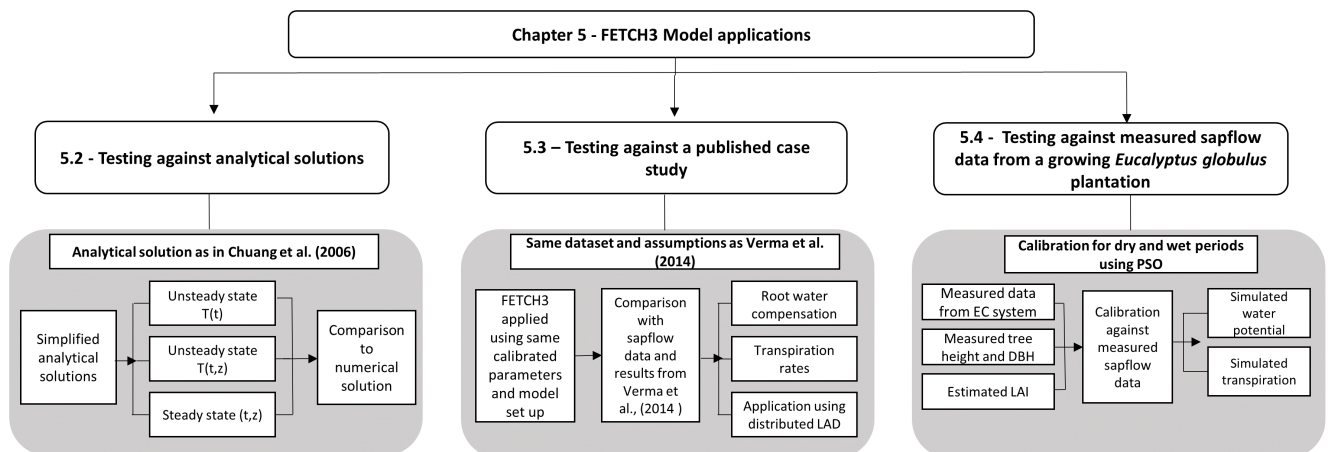


Figure 5.1: Summary of model applications described in the chapter.

5.2 Testing against analytical solutions

The numerical scheme was tested against three simplified cases that permit the derivation of solutions in closed form. Because of the nonlinear nature of the Richardson-Richards equation, only a few exact solutions are available, particularly when including sink and source terms (Broadbridge et al., 2017). An exact solution of the combined soil-to-air system (Eqs. 4.6 - 4.10) is thus too challenging to be derived. Therefore, the numerical scheme was tested against one of the equations. Eq. (4.10) was selected for this exercise and it was re-written as

$$\frac{\partial}{\partial t} (A_x \theta_x) = \frac{\partial}{\partial z} \left(A_x K_x \frac{\partial \Phi_x}{\partial z} \right) + \frac{\partial}{\partial z} (A_x K_x \rho g) - S_x, \quad (5.1)$$

where $S_x = l_a T$, with $T = T(\Phi_x, z, t)$ (m s^{-1}) the transpiration rate, and $l_a = l A_s$ (m) the leaf area per unit of height; z (m) is bound between 0 at the bottom of the tree and L at the top of the tree.

For analytical tractability of Eq. (5.1), simplified formulations of the hydraulic conductivity and water capacitance are used. The hydraulic conductivity is assumed to decrease with the water potential following the vulnerability curve (Bohrer et al., 2005; Chuang et al., 2006)

$$K_x = K_m e^{\alpha_0 \Phi_x}, \quad (5.2)$$

with α_0 (Pa^{-1}) an empirical constant and K_m ($\text{m}^2 \text{s}^{-1} \text{Pa}^{-1}$) the maximum hydraulic conductivity. Eq. (5.2) implies that $d\Phi_x = dK_x / (\alpha_0 K_x)$. The xylem water content is assumed to depend on Φ according to

$$\theta_x = \theta_{res,x} + (\theta_{sat,x} - \theta_{res,x}) e^{\alpha_0 \Phi_x}, \quad (5.3)$$

with $\theta_{res,x}$ (-) and $\theta_{sat,x}$ (-) being the residual and maximum water content of the stem xylem.

With the further assumption that $A_x = A_0 \exp(-\beta z)$, with β (m^{-1}) an empirical allometric parameter, Eq. (5.1), can be re-written as

$$\gamma_0 \frac{\partial K_x}{\partial t} = \frac{1}{\alpha_0} \frac{\partial^2 K_x}{\partial z^2} + \left(\rho g - \frac{\beta}{\alpha_0} \right) \frac{\partial K_x}{\partial z} - \rho g \beta K_x - l_a T e^{\beta z}, \quad (5.4)$$

where $\gamma_0 = (\theta_{sat,x} - \theta_{res,x}) / K_m$, (s Pa m^{-2}). Eq. (5.4) is similar to the equation described in Chuang et al. (2006), and more details regarding its derivation can be found in this study.

Assuming that at time $t = 0$ the water potential is $\Phi_x(z, 0)$, the initial condition for Eq. (5.4) reads

$$K_x(z, 0) = K_m e^{\alpha_0 \Phi_x(z, 0)}. \quad (5.5)$$

The boundary condition at the bottom of the tree is defined by a time series of water potentials (i.e., $\Phi_0 = \Phi_x(0, t)$), which results in

$$K_x(0, t) = K_m e^{\alpha_0 \Phi_0(t)}. \quad (5.6)$$

The flux of water at the top of the tree ($z = L$) is zero, leading to the boundary condition

$$\left(\frac{1}{\alpha_0} \frac{\partial K_x}{\partial z} + K_x \rho g \right)_{z=L} = 0. \quad (5.7)$$

Solutions of Eq. (5.4) with initial and boundary conditions in Eqs. (5.5) - (5.7) can be obtained for different expressions of $T(z, t)$ for some cases as presented in the following sections.

5.2.1 Simplified unsteady case

An exact solution of Eq. (5.4) can be obtained by assuming $\beta = 0$ and considering that the gradient of water potentials is the main contributor to the water fluxes (i.e., neglecting the term $\partial_z(A_x K_x \rho g)$ in Eq. 5.1)). With these assumptions, Eq. (5.4) becomes a linear diffusion equation with a sink term that can be re-written in compact form as $f_x(z, t) = l_a T$ and the boundary condition at the top of the tree reading $(\partial_z K_x / \alpha_0)_{z=L} = 0$.

A general solution of this equation can be written as (Polyanin, 2001)

$$K_x(z, t) = \int_0^L K_x(\xi, t) G(z, \xi, t) d\xi + \frac{1}{\gamma_0 \alpha_0} \int_0^t K_x(0, \tau) \left[\frac{\partial}{\partial \xi} G(x, \xi, t - \tau) \right]_{\xi=0} d\tau + \int_0^t \int_0^L f_x(\xi, \tau) G(z, \xi, t - \tau) d\xi d\tau, \quad (5.8)$$

where

$$G(x, \xi, t) = \frac{2}{L} \sum_{n=0}^{\infty} \sin \left[\frac{\pi(2n+1)x}{2L} \right] \sin \left[\frac{\pi(2n+1)\xi}{2L} \right] \exp \left[-\frac{\pi^2(2n+1)^2 t}{4L^2 \gamma_0 \alpha_0} \right]. \quad (5.9)$$

For a case where transpiration depends only on time, the sink is expressed as

$$f_x = T_m (1 - \cos(2\pi t/24)), \quad (5.10)$$

where T_m is the maximum transpiration rate, t is considered to be in hours, and it is assumed that $l_a = 1 \text{ (m}^{-1}\text{)}$.

A fixed potential, equal to 0 MPa, was considered at the bottom of the stem and along the vertical direction as initial condition. This solution was tested for a 6 m high tree with the

parameters listed in Table 5.1. Comparisons between the exact and numerical solutions using the sink term in Eq. (5.10) are shown in Figure (5.2). The errors associated with the numerical solution are small, reaching a maximum of approximately $0.25 \cdot 10^{-3}$ MPa at the top of the tree. The error followed the pattern of transpiration, reaching its peak during day time and corresponding to a maximum error of 0.09% of the exact solution. The mass balance error equalled 0.05% of the total water entering the tree during the simulated 2 days. Similarly, the lowest error could be observed at night, when transpiration approaches zero. The numerical solution presents errors that change periodically. After the influence of the initial condition disappears, the errors remain stable in time.

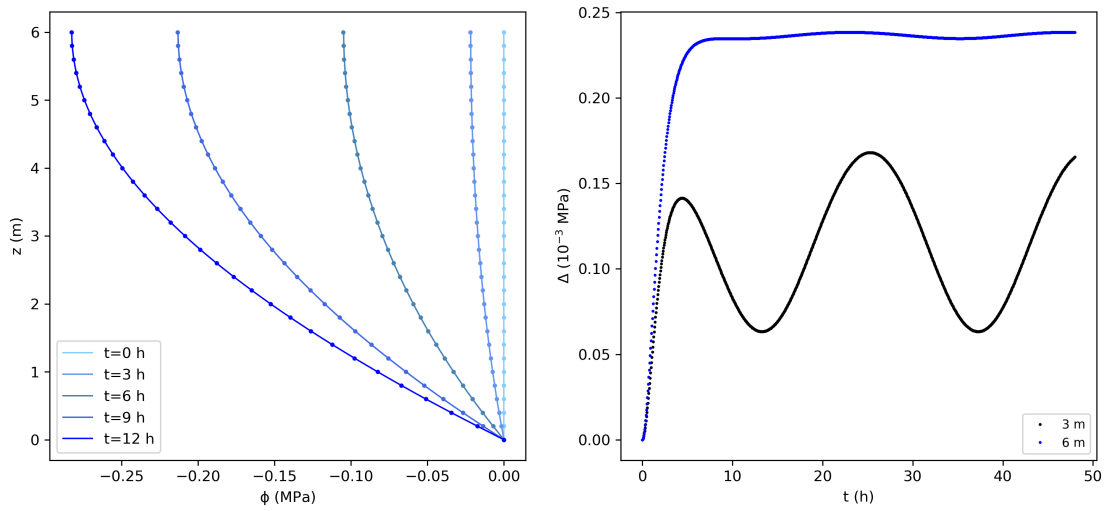


Figure 5.2: Left: water potentials (MPa) from the exact (lines) and numerical solutions (dots) using the sink term in Eq. (5.10) for the first 12 hours. For better visualization not all points are shown for the numerical solution. Right: difference between the exact and numerical solution (Δ) at 3 m and 6 m. The temporal and spatial resolutions are 0.05 h and 0.01 m, respectively.

For a case where transpiration depends on both time (t) and the vertical position (z), the sink is written as

$$f_x = T_m z (1 - \cos(2\pi t/24)), \quad (5.11)$$

where $l_a = z$ (m^{-1}).

Comparisons between the analytical and numerical solutions using Eq. (5.11) are shown in Figure 5.3, where 0 MPa was assumed at the bottom of the tree and as initial condition along the vertical direction. The error for this case is higher than for the previous case, with a maximum value that is about 0.2% of the exact solution, with a mass balance error equal to 0.05% of the total water entering the tree during the simulated 2 days. These errors would reduce using smaller values of Δz .

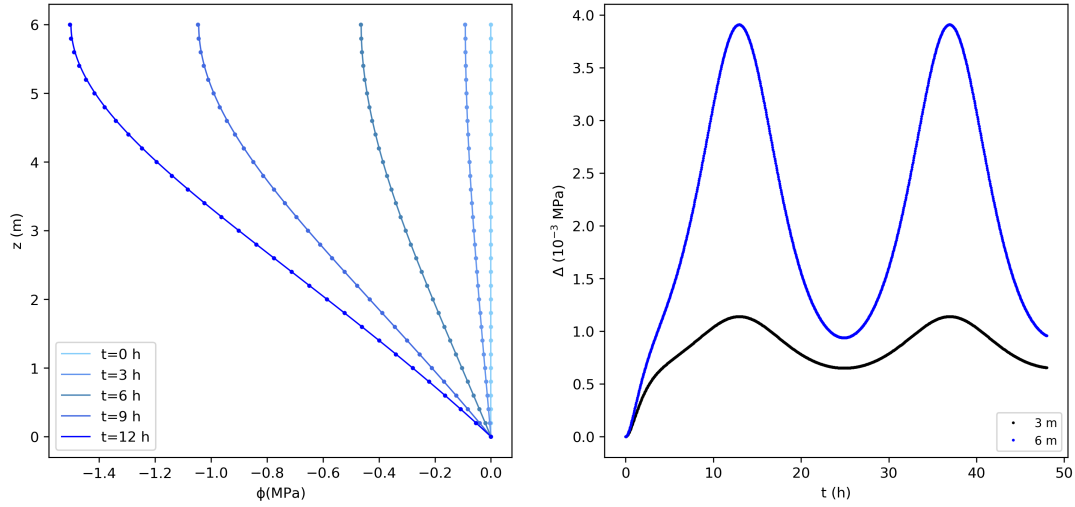


Figure 5.3: Left: water potentials (MPa) from the exact (lines) and numerical solutions (dots) using the sink term in Eq. (5.11) for the first 12 hours. For better visualization not all points are shown for the numerical solution. Right: difference between the exact and numerical solution (Δ) at 3 m and 6 m. The temporal and spatial resolutions are 0.05 h and 0.01 m, respectively.

5.2.2 Steady-state solution

A solution of Eq. (5.4) at steady state can be obtained accounting for effects due to gravity and using a distribution of leaf area per unit of stem height. It is assumed that the leaf area per unit of height is compatible with Eq. (5.4) and satisfies $l_a(0) = 0$; a possible expression for $l_a(z)$ is

$$l_a(z) = \frac{l_m \beta_1}{\beta_2 - \beta_1} \left(\frac{\beta_2}{\beta_1} \right)^{\frac{\beta_2}{(\beta_2 - \beta_1)}} \left(e^{-\beta_1 z} - e^{-\beta_2 z} \right), \quad (5.12)$$

with $\beta_2 > \beta_1$. It is also assumed that the transpiration rate depends on the water potential and the elevation as

$$T = T_m e^{\alpha_0 \Phi_x} e^{\beta_1 - \beta}. \quad (5.13)$$

Accordingly, Eq. (5.4) at steady state reads

$$\frac{1}{\alpha_0} \frac{\partial^2 K_x}{\partial z^2} + \left(\rho g - \frac{\beta}{\alpha_0} \right) \frac{\partial K_x}{\partial z} - \rho g \beta K_x + \zeta (e^{-\eta-1}) K_x = 0, \quad (5.14)$$

where $\eta = \beta_2 - \beta_1 > 0$ and

$$\zeta = \frac{l_m T_m \beta_1}{A_0 K_m (\beta_2 - \beta_1)} \left(\frac{\beta_2}{\beta_1} \right)^{\beta_2 / (\beta_2 - \beta_1)}. \quad (5.15)$$

If it is assumed that the water potential initially has a generic profile and at the bottom of the tree remains constant in time, the water potential will stabilize in time to a steady profile with the

Table 5.1: List of parameters used in the comparison between the exact and numerical solutions (section 3.1)

Parameters	Value	Units	Description
β	0	m^{-1}	Allometric parameter, vertical reduction rate of cross-sectional area
β_1	0.2	m^{-1}	Empirical shape parameter for vertical leaf area distribution per unit xylem lenght
β_2	1	m^{-1}	Empirical shape parameter for vertical leaf area distribution per unit xylem lenght
l_m	0.2	m	Mean leaf area per unit of length
A_0	0.0045	m^2	Basal cross-sectional area of the stem xylem
T_m	$3.47 \cdot 10^{-8}$	m s^{-1}	Maximum transpiration rate
α_0	$5 \cdot 10^{-7}$	Pa^{-1}	Empirical constant
$\theta_{res,x}$	0.1	-	Residual water content of the stem xylem
$\theta_{sat,x}$	0.6	-	Saturated water content of the stem xylem
K_m	$1.02 \cdot 10^{-9}$	$\text{m}^2 \text{s}^{-1} \text{Pa}^{-1}$	Maximum hydraulic conductivity

flux of water from the bottom of the tree equalling the flux of water being lost via transpiration.

The solution of Eq.(5.14) can thus be written as

$$K(z) = C_1 y^{(\alpha_0 - \beta)/\eta} J_v(y) + C_2 y^{(\alpha_0 - \beta)/\eta} Y_v(y), \quad (5.16)$$

where $J_v(.)$ and $Y_v(.)$ are the Bessel functions of the first and second kind (Abramowitz and Stegun, 1964) of order

$$v = \frac{[4\alpha_0\zeta + (\alpha_0 + \beta)^2]^{1/2}}{\eta}, \quad (5.17)$$

and C_1 and C_2 are constants to be determined numerically by imposing the boundary conditions, as in Eqs. (5.6) and (5.7) with Φ_0 constant.

The agreement between the exact and numerical solutions is shown in Figure (5.4), for a case considering a bottom boundary condition of $\Phi_0=0$ MPa, a no-flux boundary condition at the top, and a hydrostatic initial condition. Steady state was reached after a short interval of about 3 hours of model time set. For a 6 meter high tree, the error of the numerical solution increases with elevation reaching approximately $0.4 \cdot 10^{-3}$ MPa at the tree top, being 0.4% of the exact value. According to the steady-state condition, the differences in storage between the last two consecutive model time steps approached zero and were equal to $-2.77 \cdot 10^{-18} \text{ m}^3$, with transpiration equalling 99.97% of the total flux entering the tree. A larger error was reached in comparison to the unsteady state solution cases due to the more complex formulation used for the steady-case scenario.

5.3 Model application: case study

FETCH3 was tested against a case study described in Verma et al. (2014). For reproducibility purposes, FETCH3 used the same model setup, environmental variables, and parameters as Verma et al. (2014), where the software COMSOL Multiphysics (Ver. 4.1) was selected to solve

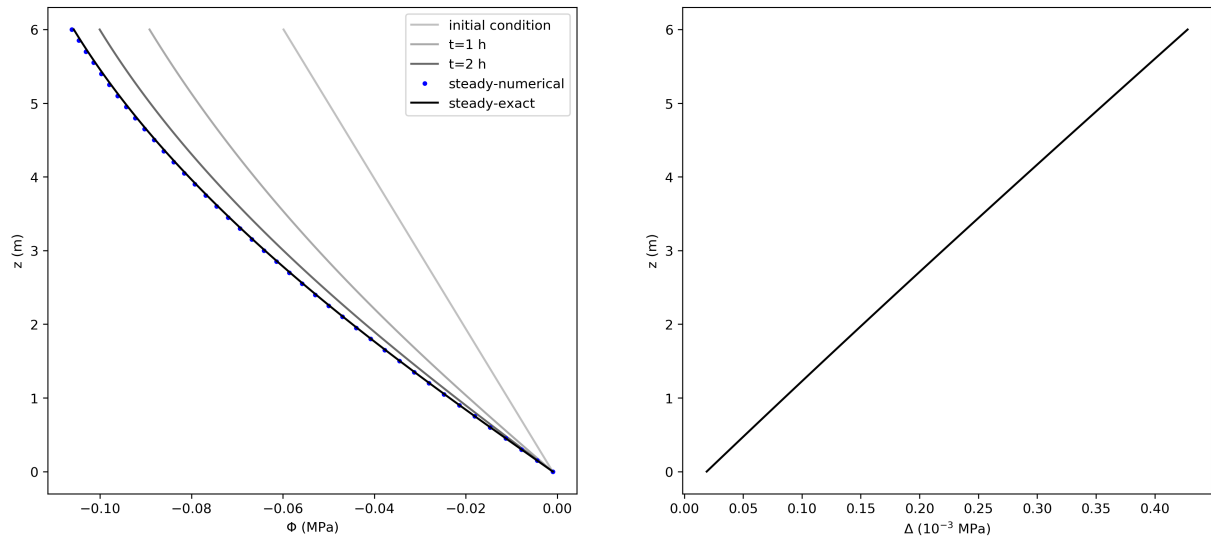


Figure 5.4: Left: water potentials, Φ , (MPa) at steady state obtained from the exact (black line) (Eq. 5.16), and numerical solutions (dots), using 0.05 m and 0.08 h as spatial and temporal resolution, respectively. For the numerical solution, not all points are shown for better visualization. The lines with light colors present the initial condition and the first 2 hours of simulation. Right: difference between the exact and numerical solution (Δ) at steady state condition along tree height.

the system of equations using finite elements. Details of the dataset are reported in Zeppel et al. (2008), Yunusa et al. (2012), and Verma et al. (2014), with a brief summary presented here.

5.3.1 Site description

The study site is located at latitude 33°39' 41" S and longitude 150°46' 57" E in New South Wales, Australia. According to the long term statistics (1993–2013 - Royal Australian Air Force base in Richmond, Australian Bureau of Meteorology, station 067105) the average daily minimum and maximum temperatures are 10 °C and 24 °C, with annual rainfall approximately 730 mm.

Rainfall, solar radiation, air temperature, and humidity were collected every 30 minutes from January 1st to June 4th in 2007. Sap flux data were collected for the same period, using the heat ratio technique at a half-hour resolution. The vegetation is dominated by *Eucalyptus parramattensis* C.A. Hall (Parramatta red gum) and *Angophora bakeri* E.C. Hall (narrow-leaved apple). The trees were 14 m tall on average, with a LAI between 1.3 and 1.9.

The soil is duplex, with a first layer up to a depth of 0.8 m being predominantly sand, with clay underneath. The soil parameters used in the model are listed in Table 5.2.

Table 5.2: List of soil parameters used in the model application

Parameters	Units	Sand	Clay	Description
$k_{s,sat}$	m s^{-1}	$3.45 \cdot 10^{-5}$	$1.94 \cdot 10^{-7}$	Saturated hydraulic conductivity
θ_{sat}	—	0.47	0.55	Saturated volumetric soil moisture content
θ_{res}	—	0.045	0.068	Residual volumetric soil water content
α	m^{-1}	14.5	0.8	van Genuchten parameter
n	—	2.4	1.5	van Genuchten parameter
θ_1	—	0.05	0.08	Root water uptake reduction function parameter
θ_2	—	0.09	0.12	Root water uptake reduction function parameter

5.3.2 Model setup

The system of equations was solved for a soil depth of 5 m, and trees with a height of 14 m and root depth of 3.2 m. The boundary condition at the soil bottom was a constant water potential equal to -0.06 MPa, corresponding to a water content of $0.28 \text{ m}^3\text{m}^{-3}$. At the surface, measured rainfall was used as a flux boundary condition to compute soil water infiltration (refer to Section 4.3.2). The boundary conditions for the trees are a zero-flux condition at the bottom of the roots and, above-ground, transpiration is applied as a boundary condition at the top of the canopy. Daytime transpiration is modelled through the Penman Monteith equation (Allen et al., 1998) combined with a stomata conductance function (Jarvis, 1976), whereas night time transpiration follows a more simplified formulation composed of a constant nighttime transpiration value modulated by temperature, VPD, and water potential at night (refer to Section 4.4). In order to follow the same setup as in Verma et al. (2014), transpiration is not distributed along the stem, but is imposed as a flux concentrated at the top of the tree, and the water capacitance of the xylem in the roots and stem is assumed constant (Verma et al., 2014).

In the sand layer, soil initial conditions are assumed to be a constant water potential equal to -0.004 MPa, corresponding to a water content of $0.08 \text{ m}^3\text{m}^{-3}$. In the clay layer, water potential below a depth of 3 m was constant and equal to -0.06 MPa. Between these two depths, water potential was interpolated linearly. For the tree, water potential linearly decreased from -0.06 MPa at the bottom of the roots to -0.22 MPa at the top of the canopy. The spatial resolution used was 0.1 m, and the time step 20 s. The list of parameters used in the model, including root water uptake and transpiration parameters, is in Table 5.3.

5.3.3 Results

The model predictions for sap-flux during the day compared well with observation during the entire measurement period (Figure 5.5a), reaching a R^2 value of 0.74. The total mass balance error in the soil represented -0.30% of total infiltration, and it was calculated as the change in soil water storage minus the difference between the flux entering (bottom boundary condition and infiltration) and exiting the soil (root water uptake). In the tree (root and stem xylem), the

Table 5.3: List of parameters used in the application of the model as in Verma et al. (2014)

Parameters	Units	Value	Description
A_x/A_s	-	$8.6 \cdot 10^{-4}$	Stem xylem cross sectional area index surface ratio
A_r/A_s	-	1	Root xylem cross sectional area index
A_{ls}/A_s	-	1	Lateral root surface area index
LAI	-	1.5	Leaf area index
$k_{s,rad}$	s^{-1}	$7.2 \cdot 10^{-10}$	Total soil-to-root radial conductance
C_x	Pa^{-1}	$1.1 \cdot 10^{-11}$	Stem xylem water capacitance
C_r	Pa^{-1}	$1.1 \cdot 10^{-11}$	Root xylem water capacitance
h	m	14	Tree height
C_p	$J m^{-3} K^{-1}$	1200	Heat capacity of air
T_{opt}	K	289.15	Jarvis temperature parameter
λ	$J m^{-3}$	$2.51 \cdot 10^9$	Latent heat of vaporization
γ	$Pa K^{-1}$	66.7	Psychometric constant
g_b	$m s^{-1}$	$2 \cdot 10^{-2}$	Leaf boundary layer conductance
g_a	$m s^{-1}$	$2 \cdot 10^{-2}$	Aerodynamic conductance
k_r	$m^2 W^{-1}$	$5 \cdot 10^{-3}$	Jarvis radiation parameter
k_t	K^{-2}	$1.6 \cdot 10^{-3}$	Jarvis temperature parameter
k_d	Pa^{-1}	$1.1 \cdot 10^{-3}$	Jarvis vapor pressure deficit parameter
h_{x50}	m	-130	Jarvis leaf water potential parameter
g_{smax}	$m s^{-1}$	$10 \cdot 10^{-3}$	Maximum leaf stomatal conductance
n_l	-	2	Jarvis leaf water potential parameter
E_{max}	$m s^{-1}$	$1 \cdot 10^{-9}$	Maximum night time transpiration
q_z	-	9	Root distribution parameter
k_{max}	$m s^{-1}$	$1 \cdot 10^{-5}$	Maximum conductivity of saturated stem xylem
k_{sax}	$m s^{-1}$	$1 \cdot 10^{-5}$	Specific axial conductivity for the root system
a_p	Pa^{-1}	$2 \cdot 10^{-6}$	Xylem cavitation parameter
b_p	Pa	$-1.5 \cdot 10^{-6}$	Xylem cavitation parameter

water mass error was -0.16% of the total infiltration, and was calculated as the change in water storage (in the stem and root xylem) minus the difference between the fluxes entering (root water uptake) and exiting (transpiration) the tree. The model maintained a continuous water potential along roots and stem xylem (Figure 5.5b). At midday, in the roots, water potential decreases almost linearly with elevation, while in the stem xylem, because of the transpiration flux at the top of the tree, it is non linear. The change in the gradient at the soil surface is due to the sharp change in the axial hydraulic conductivity, since the xylem cross-sectional area index for the stem ($A_x/A_s=8.6 \cdot 10^{-4}$) is different from that of the roots ($A_r/A_s=1$).

For the days shown in Figure 5.5b, when transpiration is peaking, the water potential fluctuates between a minimum of -2.2 MPa at the tree top and -0.8 MPa at the bottom of the roots. This range of values is in agreement with the results from the original studies and the published literature (Choat et al., 2012; Franks et al., 2007; Quijano and Kumar, 2015; Verma et al., 2014).

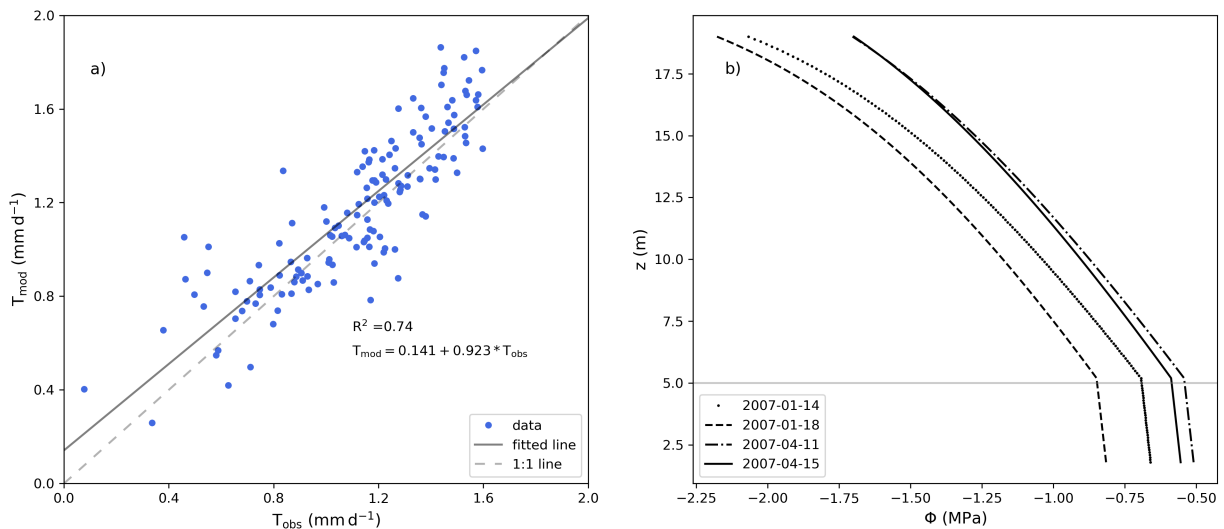


Figure 5.5: a) Comparison between measured (T_{obs}) and modelled (T_{mod}) daily sap flux rates excluding fluxes during the night. b) Root and stem xylem water potential (MPa) as a function of elevation (z) at midday. The vertical position of 5 m (above $z=0$, which is defined as the bottom of the soil column) represents the interface between between the roots and the stem.

A comparison of modelled and observed time series of transpiration rates for a week in January (summer) and April (autumn) is shown in Figure 5.6. The model is able to reproduce the temporal patterns of transpiration during the day, and does not show large fluxes at night because of the simplified modelling of the stomatal conductance at night, as in Verma et al. (2014) (see Section 4.4).

FETCH3 was able to accurately represent the nonlinear interactions between the above- and below-ground components of the SPAC. From Figure 5.6, we can verify that root water uptake and transpiration are coupled, meaning that below-above ground interface is correctly repres-

ented by the model. Below-ground, shallow soil layers generated maximum rates of root water uptake (RWU) during most days, caused by greater root density and low water stress when water is readily available. During dryer days, with the decrease of soil moisture at the surface, considerable RWU was found in the deeper layers (approximately 20 - 30 cm from the soil surface). Root water uptake from deeper layers can be characterized as a hydraulic compensation path generated by rapid reductions in the top layers radial hydraulic conductivity, as it can be seen in Figure 5.6a, during the last 3 days in January.

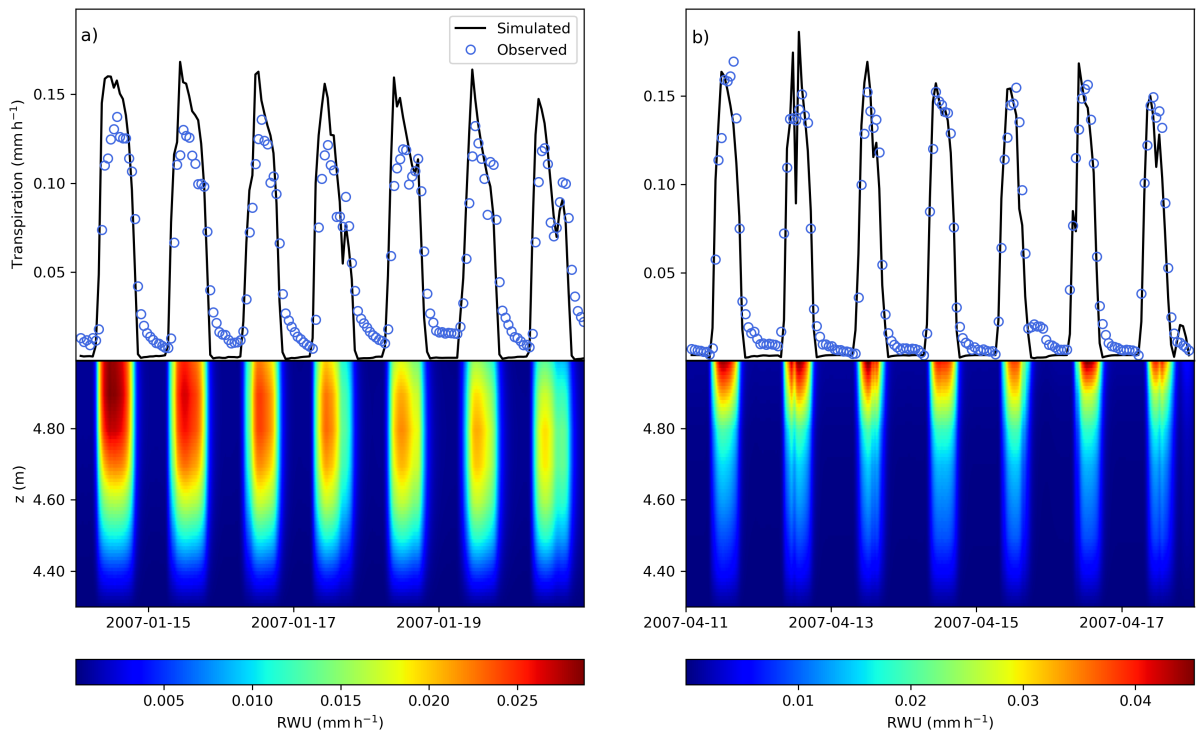


Figure 5.6: Comparison between modelled (black line) and observed (blue circles) transpiration rates and modelled root water uptake (colormap, mm h^{-1}) during one-week periods in (a) January and in (b) April. The vertical position of 5 m (above $z=0$, which is defined as the bottom of the soil column) represents the interface between the roots and the above-ground stem xylem.

5.4 Modelling LAD and water capacitance

FETCH3 is able to simulate the distribution of transpiration along the vertical axis, as well as a water capacitance function for the roots and stem xylem. In order to test this capability, we applied FETCH3 using the same parameters and setup as in section 5.3.2, but changed how the transpiration and xylem water capacitance are modelled in the case study. For this experiment, transpiration is not a boundary condition at the tree top, but is distributed along the stem as in Eq. (4.10), with S_x/A_s depending on the leaf area density (LAD). At the tree top, a

no-flux condition is applied. An empirical LAD function described in Lalic and Mihailovic (2004) was used, and a LAD profile suitable for *Eucalyptus* stands can be written as:

$$l(z) = l_{max} \left(\frac{h - z_m}{h - z} \right)^{n_0} \exp \left[n_0 \left(1 - \frac{h - z_m}{h - z} \right) \right], \quad (5.18)$$

where h is the tree height (m), l_{max} ($\text{m}^2 \text{m}^{-3}$) is the maximum value of leaf area density in a layer, z_m (m) is the corresponding above-ground height of l_{max} , and n_0 (-) is an empirical parameter defined as

$$n_0 = \begin{cases} 6 & 0 \leq z < z_m, \\ 0.5 & z_m \leq z \leq h. \end{cases} \quad (5.19)$$

The value of l_{max} can be calculated from the LAI imposing

$$LAI = \int_0^h l(z) dz. \quad (5.20)$$

Following Chuang et al. (2006) and Bohrer et al. (2005), the water capacitance of the roots and stem xylem are

$$C_x(\Phi_x) = \frac{A_x}{A_s} \frac{\partial \theta_x}{\partial \Phi_x} = \frac{A_x p \theta_{sat,x}}{A_s \Phi_d} \left(\frac{\Phi_d - \Phi_x}{\Phi_d} \right)^{-(p+1)}, \quad (5.21)$$

$$C_r(\Phi_r) = \frac{A_r}{A_s} \frac{\partial \theta_r}{\partial \Phi_r} = \frac{A_r p \theta_{sat,r}}{A_s \Phi_d} \left(\frac{\Phi_d - \Phi_r}{\Phi_d} \right)^{-(p+1)}, \quad (5.22)$$

where Φ_d (Pa) and p (-) are empirical coefficients for the hydraulic system, and $\theta_{sat,x}$ (-) and $\theta_{sat,r}$ (-) are the water content at saturation for the stem and roots xylem, respectively. The values of these parameters are shown in Table 5.4.

From Figure 5.7, the vertical distribution of transpiration follows the shape of the LAD, with larger values of transpiration where the LAD is also large. Accordingly, Φ decreases along the tree height, in accordance with the no-flux boundary condition applied at the top of the tree.

5.5 Model application: calibration against measured sap flux data

FETCH3 was calibrated against sap flow data collected in the young blue gum plantation described in Chapter 3, referred here as Digby plantation. For these simulations, FETCH3 used the environmental variables collected at the site as input to run the model.

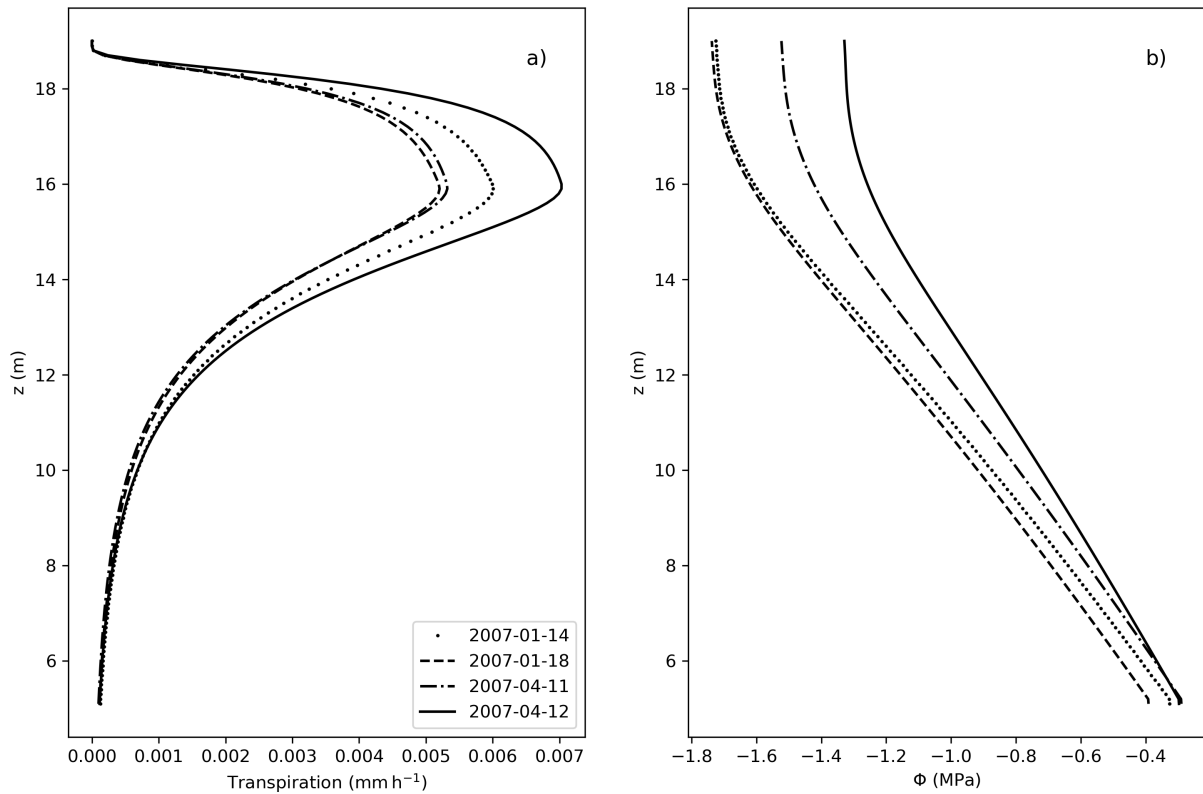


Figure 5.7: a) Transpiration fluxes (mm h^{-1}) as a function of the elevation (z). b) Water potential (MPa) along z , considering $z=0$ at the bottom of the soil, and $z=5$ m equal the bottom of the stem.

5.5.1 Data description

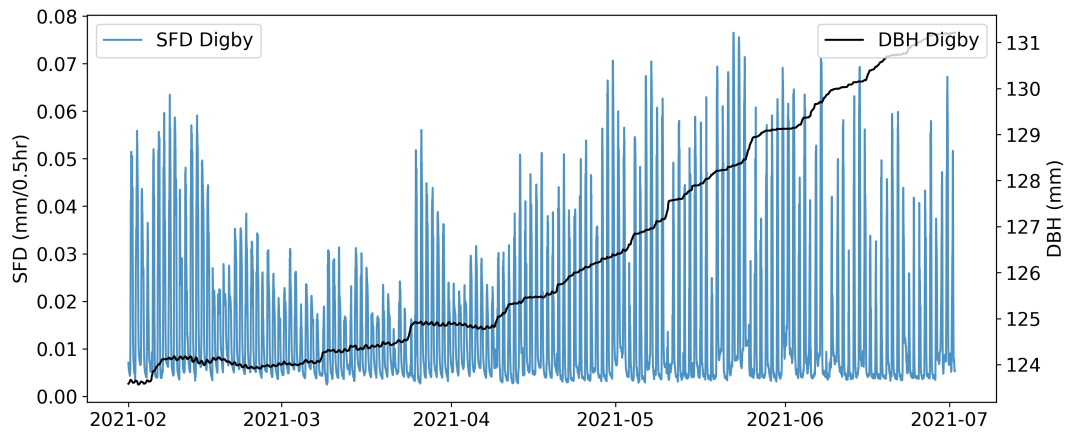
Transpiration was measured in individual trees using commercially available sap flow sensors (SFM1, ICT International, Australia). The SFM1 uses the heat pulse velocity (HPV) technique to measure sap flow rates from the velocity of a short pulse of heat moving along the xylem tissue. Sap flow sensors were installed approximately at breast height in 5 trees and HPV recorded at half-hourly intervals. Velocities were corrected for wounding effects following Burgess et al. (2001), using compatible values for *Eucalyptus* trees from the literature (Burgess et al., 2001; Choat et al., 2012; Fraser, 2020). Additional measurements of tree diameter at breast height (DBH) were performed by dendrometers (DBL60, ICT International, Australia) installed on the same trees. Stem diameter variations were recorded every 30 minutes. Given that plantation trees are generally homogeneous and equally spaced, the measured trees were assumed to be representative of the entire plantation.

Measurements were converted to sap flux density (SFD, $\text{m}^3\text{m}^{-2}\text{h}^{-1}$), based on wood core measurements of dry wood density, gravimetric sapwood moisture content, and sapwood area. For the plantation, sapwood area was assumed to be the entire stem, as it is commonly the case for young *Eucalyptus* trees (Benyon and Doody, 2015; Drake et al., 2012), and also verified

Table 5.4: List of parameters used in the application of the model considering a water capacitance and a leaf area density function

Parameters	Units	Value	Description
l_{max}	m^2m^{-3}	0.4	Maximum value of leaf area density
z_m	m	11	Corresponding above-ground height of l_{max}
n_0	-	6 or 0.5	Empirical parameter (Eq. 5.19)
Φ_d	Pa	$5.74 \cdot 10^8$	Empirical parameter for water pressure of dry xylem
p	-	20	Empirical coefficient
$\theta_{sat,x}$	-	0.58	Water content at saturation for the stem xylem
$\theta_{sat,r}$	-	0.58	Water content at saturation for the root xylem

during the core sampling. From average SFD, plot-level transpiration (mm h^{-1}) was obtained using the total sapwood area calculated based on the measurements of DBH, following Kume et al. (2010) and Marchionni et al. (2019). Figure 5.8 shows the plot-level transpiration and diameter change. The measurement period was 2nd of January 2021 to 1st of July 2021.

**Figure 5.8:** Sap flux density (SFD) and diameter at breast height (DBH) during the monitored period.

5.5.2 Model setup

A 5 m deep sandy-loam soil layer was considered in the model, following Dresel et al. (2018). The boundary condition at the soil bottom was constant water potential equal to $-3.06 \cdot 10^{-4}$ MPa, corresponding to a water content of $0.30 \text{ m}^3\text{m}^{-3}$. At the surface, measured rainfall was used as a flux boundary condition to compute soil water infiltration, considering a constant interception of 20% of rainfall. The percentage of interception was derived using an equation described in Amenu and Kumar (2007), which considers the average LAI of the site to calculate the amount of water intercepted by leaves. The boundary conditions for the trees were a zero-flux condition at the bottom of the roots and, above-ground, a zero-flux condition applied at the top of the tree. Transpiration is modelled as in Section 5.4, with transpiration and capacitance

Table 5.5: List of parameters values used in the application of FETCH3 for the Digby plantation

Parameters	Units	Value	Reference
Tree density	trees hec^{-1}	750	Measured
Plot area	m^2	10000	Measured
Mean sapwood area	m^2	$1.2 \cdot 10^{-2}$	Measured
A_x/A_s	-	$1.2 \cdot 10^{-3}$	Estimated from sapwood area
A_r/A_s	-	$1.2 \cdot 10^{-3}$	Estimated from sapwood area
A_{ls}/A_s	-	1	Estimated from sapwood area
LAI	-	2	Estimated from allometric equations
h	m	9	Measured
C_p	$\text{J m}^{-3} \text{K}^{-1}$	1200	From Vermaet al. (2014)
T_{opt}	K	293.65	from Vermaet al. (2014)
λ	J m^{-3}	$2.51 \cdot 10^9$	From Vermaet al. (2014)
γ	Pa K^{-1}	66.7	From Vermaet al. (2014)
g_b	m s^{-1}	$2 \cdot 10^{-2}$	From Vermaet al. (2014)
g_a	m s^{-1}	$2 \cdot 10^{-2}$	From Vermaet al. (2014)
k_r	$\text{m}^2 \text{W}^{-1}$	$5 \cdot 10^{-3}$	From Vermaet al. (2014)
k_t	K^{-2}	$1.6 \cdot 10^{-3}$	From Vermaet al. (2014)
k_d	Pa^{-1}	$1.1 \cdot 10^{-3}$	From Vermaet al. (2014)
n_l	-	2	From Vermaet al. (2014)
E_{max}	m s^{-1}	$1 \cdot 10^{-8}$	From Vermaet al. (2014)
q_z	-	12	Adapted from Vermaet al. (2014)
k_{max}	m s^{-1}	10^{-8}	Adapted from Vermaet al. (2014)
k_{sax}	m s^{-1}	10^{-8}	Adapted from Vermaet al. (2014)
θ_{sat}	-	0.41	From vanGenuchten (1980)
θ_{res}	-	0.065	From vanGenuchten (1980)
α	m^{-1}	7.5	From vanGenuchten (1980)
n	-	1.89	From vanGenuchten (1980)
θ_1	-	0.02	Adapted from Vermaet al. (2014)
θ_2	-	0.2	Adapted from Vermaet al. (2014)

distributed along the stem.

For the soil, initial conditions were assumed to be a soil water potential of -0.01 MPa corresponding to a water content of $0.12 \text{ m}^3 \text{m}^{-3}$ for the first 80 cm from the surface. Below a depth of 3.6 m, soil water potential was constant and corresponding to $0.28 \text{ m}^3 \text{m}^{-3}$. Between these two depths, water potential was interpolated linearly. Initial conditions for the trees consisted in water potential hydrostatically decreasing from the bottom of the roots to the top of the stem, assuming that the bottom of the roots has the same water potential as the soil at the same depth. A root depth of 1.2 m and a tree height of 9 m were set. Parameters were estimated from the literature on *Eucalyptus globulus* trees (Barotto et al., 2017; Barrett et al., 2005; David et al., 1997; Drake et al., 2009, 2012; Franks et al., 2007) and from plant physiology and traits databases (Choat et al., 2012; Falster et al., 2015; Fraser, 2020; Pausas et al., 2016), and are listed in Table 5.5. The spatial resolution used was 0.1 m, and the time step 20 s.

5.5.3 Automatic calibration using PSO

The methodology chosen for the calibration was the Particle Swarm Optimization (PSO) (Kennedy and Eberhart, 1995). PSO is a heuristic optimization method and a bio-inspired algorithm, mimicking the collective behavior of a flock of birds or a swarm of bees. In this approach, a population of particles, representing individual solutions to the problem, moves through the solution space by performing multiple iterations until they converge to an optimal solution of an objective function (Scheerlinck et al., 2009). For this study, PSO was applied using PySwarms (<https://pyswarms.readthedocs.io/>, accessed 31/03/2022), a widely used Python-based tool.

PSO requires the definition of the objective function. For the calibration, the root mean square error (RMSE) was chosen, as

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n}}, \quad (5.23)$$

with n the number of data points, y the observed sap flux data and $\hat{y}$ the simulated transpiration data. In this application, the overall RMSE was calculated based on the half-hourly values of the variables, excluding nighttime data. PSO performed consecutive simulations of FETCH3 until the difference in the RMSE function between simulations was less than $10^{-8} \text{ mm } 0.5\text{h}^{-1}$. The parameters chosen for the calibration were $k_{s,rad}$, g_{smax} , a_p , b_p , h_{x50} , and $k_{s,sat}$. These parameters were chosen based on the model sensitivity, and because they represent plant-functional traits, such as resistance to cavitation and root uptake behavior. With the exception of $k_{s,sat}$ the calibrated parameters can express considerable differences according to plant species, age, site climate, and management practices (Matheny et al., 2017; Pappas et al., 2016). The parameter $k_{s,sat}$ is associated with a physical property of the soil, and should be independent of soil moisture. However, given the high spatial variability of soil properties, which can change over only a few centimetres (Manzoni et al., 2013b), $k_{s,sat}$ was calibrated separately for the two periods of time under analysis.

PSO requires the definition of an upper and lower bound for each parameter that will be calibrated. The upper and lower bounds chosen were based on values for blue gum trees found in the databases described in Choat et al. (2012), Falster et al. (2015), and Fraser (2020). The dataset was divided into dry (February - March 2021) and wet (May - June 2021) periods. Table 5.6 contains the resultant parameters for each period after calibration using PSO.

5.5.4 Results

Table 5.7 shows the calibration period, RMSE for the calibration, and the R^2 for the simulation period. The calibrated parameters during the wet period generated good predictions of transpir-

Table 5.6: List of calibrated values of parameters for each simulation

Parameters	Units	Dry period	Wet period
$k_{s,rad}$	s^{-1}	$1.30 \cdot 10^{-13}$	$3.26 \cdot 10^{-11}$
g_{smax}	$m s^{-1}$	$2.04 \cdot 10^{-2}$	$2.09 \cdot 10^{-2}$
a_p	Pa^{-1}	$1.70 \cdot 10^{-6}$	$3.45 \cdot 10^{-7}$
b_p	Pa	$-1.00 \cdot 10^5$	$-1.33 \cdot 10^6$
h_{x50}	m	$-1.17 \cdot 10^5$	$-2.11 \cdot 10^6$
$k_{s,sat}$	$m s^{-1}$	$1.11 \cdot 10^{-5}$	$1.27 \cdot 10^{-5}$

ation that compared well with the measured sap flow from Digby over the same period. During May and June 2021, the R^2 for the daily transpiration, excluding nighttime values, was 0.66 (Figure 5.9, b), which is close to the value registered for the case study from Verma et al. (2014). The RMSE for the calibration period was small, considering that it was lower than the standard deviation of the dataset, which was $0.0164 \text{ mm } 0.5h^{-1}$. Looking at the simulated hourly rates, FETCH3 predictions overestimated transpiration during the majority of May (Figure 5.9, c), but reached good agreement in June (Figure 5.9, a).

Table 5.7: Calibration and Simulation period, with the respective RMSE ($\text{mm } 0.5h^{-1}$) from the calibration with PSO and R^2 for the simulation period.

Simulation	Dry period	Wet period
Calibration period	07 Feb - 07 Mar	26 May - 26 Jun
RMSE calibration	$9.50 \cdot 10^{-3}$	$1.33 \cdot 10^{-2}$
Simulation period	01 Feb - 01 Apr	01 May - 01 Jul
R^2 simulation	0.43	0.66

During the dry period, even though the RMSE was still smaller than the standard deviation of the calibration dataset ($0.0127 \text{ mm } 0.5hr^{-1}$), the results were not as good as during the wet period, registering a R^2 of 0.43 (Figure 5.10, b). FETCH3 was not able to replicate completely the water stress in March 2021 (Figure 5.10, a), and overestimated transpiration during most of this period. Contrarily, during early February, the model underestimated transpiration (Figure 5.10, c).

The considerable growth over the monitored period, especially during winter, made it harder to derive a single set of calibrated parameters for the site, since tree DBH from February (124 mm) was considerably smaller than in June (132 mm). The increasing DBH influenced the calculation of the sap flux density over time. This made it challenging for FETCH3 to reproduce the behavior of the trees, giving that the current version of the model does not account for tree growth (above and below ground) or variation in sapwood area during simulations. Additionally, the high variability in DBH over a short period of time might have increased the uncertainties in the calculation of the plot-scale sap flux density. Uncertainties and errors in the data also play a role. Potential errors in measurement of SFD using the HPV method may include up to 35% underestimation of the actual SFD after corrections. Errors can increase with SFD

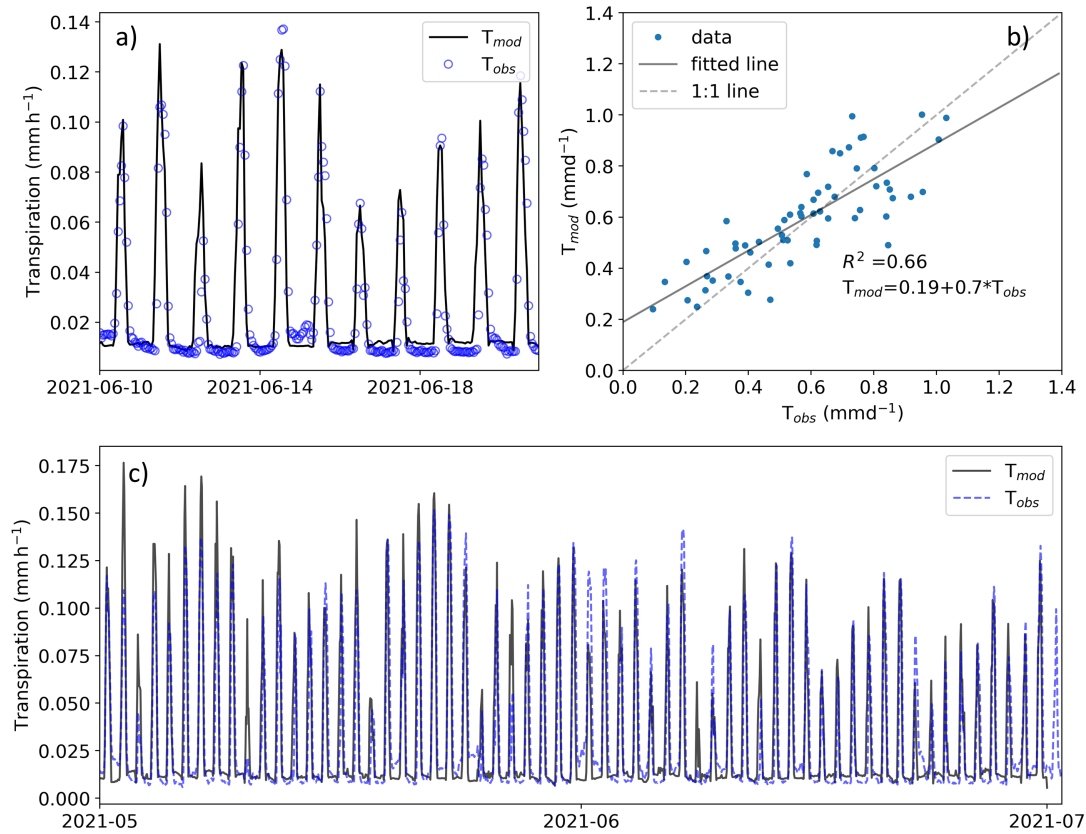


Figure 5.9: Results for the wet period: a) comparison between measured (T_{obs}) and modelled (T_{mod}) sap flux rates for a period of 10 days in June, b) comparison between T_{obs} and T_{mod} daily sap flux rates for the entire simulation period excluding fluxes during the night, and c) comparison between T_{obs} and T_{mod} for the entire simulation period.

due to sap wood heterogeneity (Steppe et al., 2010). In addition, SFD measurements do not account for the lag in water withdrawn from storage, which can account for 10 to 15% of the daily transpiration (Matheny et al., 2015).

The high sap flux during winter (when compared to summer) and the large sap flux variability over summer at the growing plantation are difficult to model with the Penman-Monteith formulation of transpiration. The Penman-Monteith formulation used here (Eq. 4.57) assumes that transpiration is proportional to net radiation and VPD, which are usually higher during summer and decrease as winter approaches (refer to Figure 3.2, Chapter 3). The young trees at Digby were constantly growing and, differently from the northern-hemisphere ecosystems, they grew considerably during winter, when it is wet in the plantation. As a result, considering the decreasing VPD and radiation during May and June, FETCH3 was not able to replicate the large transpiration variability from February to July as a single simulation. Additionally, the current version of FETCH3 applies a simplified night-time transpiration function, which may have also contributed to the poor performance of the model during summer. Despite the limitations, FETCH3 reached a R^2 of 0.66 during the wet period.

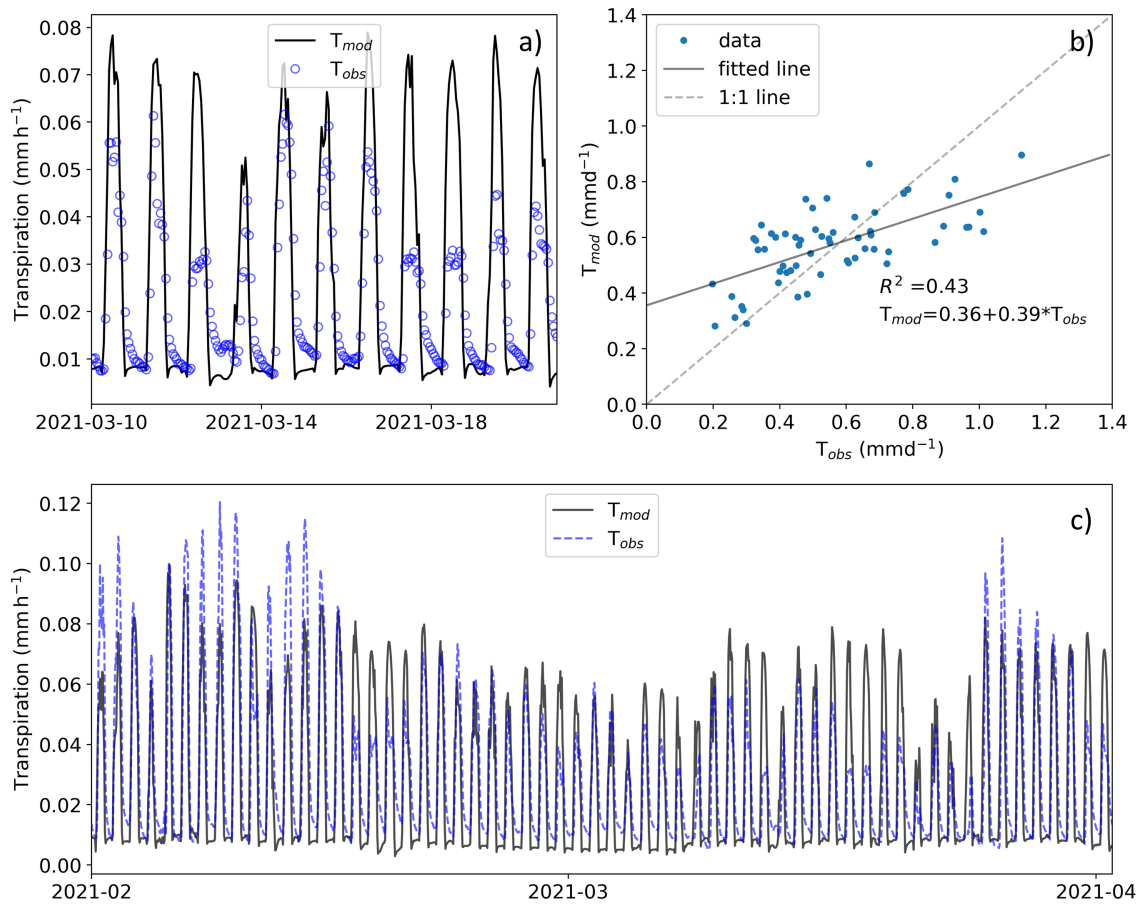


Figure 5.10: Results for the dry period: a) comparison between measured (T_{obs}) and modelled (T_{mod}) sap flux rates for a period of 10 days in March, b) comparison between T_{obs} and T_{mod} daily sap flux rates for the entire simulation period excluding fluxes during the night, and c) comparison between T_{obs} and T_{mod} for the entire simulation period.

Applying the same model set up for both dry and wet periods, only changing the five calibrated parameters, may also have contributed to the lower R^2 registered for the dry period. Even though blue gum trees are considered an evergreen species, the seasonal variation in LAI can be substantial and cause different interception rates, also affecting the root water uptake capacity (Battaglia et al., 1998; White et al., 2010). This variation can be even larger for young trees, as considerable stand development, below and above ground, can occur in a few months period (for example, DBH variation in Figure 5.8). As a result, differences in tree development and traits, when comparing the wet and dry period, were not included, likely affecting the model performance. For example, θ_1 , θ_2 , and q_z were the same for dry and wet periods, even though root water uptake capacity and resistance to water stress are highly dependent on tree development and photosynthesis capacity (influenced by the LAI) (Christoffersen et al., 2016; Matheny et al., 2017; Pereira et al., 1997); this might have resulted in contrasting results. This can be seen around mid March, when the sap flux data shows a reduction in transpiration not replicated by FETCH3, which consistently overestimated the sap flow rates during the drier days.

Therefore, general model set up and parameters might have been a better fit to the wet period, resulting in improved results for May - July.

5.6 Conclusions

The Finite-difference Ecosystem-scale Tree Crown Hydrodynamics version 3 (FETCH3) was tested and applied in this study. By using a porous-media approach, FETCH3 is able to simulate intradaily dynamics of transpiration and provides a fast response to environmental variables. FETCH3 allows fidelity in the representation of hydraulic traits, which can be used to explore plant responses to water stress and xylem processes rather than land-atmosphere interactions.

We tested FETCH3 against exact numerical solutions of the equations and observations of transpiration. The numerical scheme of the model was applied to two simplified exact non-steady state cases, reaching a maximum error of approximately 0.2% with respect to the exact solution at the tree top of a 6 m high tree, for a case in which transpiration is dependent on both time and elevation. For a steady-state scenario, considering a more complex formulation, the error approached 0.4% of the exact solution at the tree top.

Simulated transpiration rates from FETCH3 reached an R^2 of 0.74 in comparison to observed sap flow rates from a published case study. In addition, values of water potential were continuous along roots and stem xylem, showing that water flux in the soil, roots, and stem are correctly coupled along the entire tree structure. By using a hydrodynamic set of equations, FETCH3 resolves the temporal and vertical dynamics of root water uptake, and stem and root water transport and storage. This allows FETCH3 to simulate hydrodynamic phenomena such as root water compensation following reductions of soil moisture in the shallow soil layers.

FETCH3 produced good results when calibrated against measured sap flow collected from a growing plantation during the wet period of May - July 2021, with a R^2 of 0.66. However, it did not performed well during a drier summer period (February and March 2021). Limitations in the application of FETCH3, for this case, included the complexity of simulating growing trees with a model formulation that does not include tree growth. Additionally, as the same model set up was applied for both periods, FETCH3 might not have been able to accurately simulate the stage of tree development during each period, given that growing trees can sharply change in only few months.

By comparing the model predictions of transpiration and soil and xylem water storage with different sets of parameters (describing the whole-tree hydraulic strategy of the trees), and different environmental forcing (describing realistic or hypothetical conditions and stress), FETCH3 allows model-based studies of the consequences of hydraulic traits and strategies of different tree species for above- and below-ground water transport, with a range of stem and root xylem hydraulic characteristics.

Chapter 6

Conclusion

In the next sections, the results of the project are summarized, the contributions of the thesis are presented, the practical implications of this project are discussed, and the future work and limitations of the project are highlighted.

6.1 Summary of results

6.1.1 Experimental work

This project quantified the water and carbon fluxes in a young *Eucalyptus globulus* plantation during its first 4 years after establishment in a site located in southwest Victoria, Australia. The fluxes were measured using the eddy covariance method with the equipment raised above the canopy as the trees grew; additional measurements of tree height and diameter at breast height were taken to monitor tree growth and provide estimations of LAI.

Measured evapotranspiration (ET) at the site did not vary considerably over the years, even though trees were growing and developing continuously. However, the Net Ecosystem Production (NEP) and Gross Ecosystem Production (GEP) substantially increased over time, with the plantation switching from being an overall carbon source to a carbon sink in approximately 2 years. Increases in carbon fluxes were a result of tree growth and development, with DBH and estimated Leaf Area Index (LAI) substantially increasing in time. The dynamics of tree growth dictated how evapotranspiration was partitioned as trees developed, with soil evaporation and understory transpiration decreasing as trees grew, as a result of increasing LAI and DBH. Therefore, although ET did not increase substantially as the trees grew, the large increase in GEP resulted in a large increase in water use efficiency (WUE) of the plantation during the monitoring period.

The different dynamics in water and carbon fluxes for young stands captured by this study high-

lighted the need to evaluate stand age and species-specific characteristics. The management practices currently applied to commercial plantations in Australia only refer to an estimated annual water use. Differently from what commonly assumed to provide licenses for plantation establishment, the plantation in our study did not see a dramatic increase in ET as the trees grew. Small increments in water used generated substantial increases in productivity, highlighting that management practices should be site specific and consider the trade-offs of water used by the trees against the gain in carbon assimilation.

6.1.2 FETCH3

The Finite-difference Ecosystem-scale Tree Crown Hydrodynamics (FETCH3) was developed. FETCH3 simulates water flowing through the soil-plant-atmosphere continuum by assuming that the water movement in the xylem resembles flow in porous media, and uses a macroscopic approach, lumping soil, roots, and stems along the vertical direction. FETCH3 solves a system of three partial differential equations in a 1D domain to describe the water flow through the soil, root xylem, and stem xylem.

FETCH3 presented a novel methodology to fully couple the soil, roots, and stem, assuring the continuity of the water fluxes between these three compartments. FETCH3 can simulate above- and below-ground water transport, accounting for root water uptake strategies, such as root water compensation and hydraulic redistribution along the vertical direction. The numerical formulation of the model was tested against exact solutions (non-steady and steady cases), transpiration observations from a published case study, and calibration was performed for the trees at the growing plantation experimental site.

The model presented considerably small errors when compared to the exact solutions and was able to correctly represent transpiration patterns when compared to experimental data from a case study that provided calibrated parameters. FETCH3 produced good results when calibrated against measured sap flow data from the growing plantation collected during the wet period, but it did not performed well during the drier period. As the model does not include a formulation to simulate tree growth, FETCH3 was not able to fully replicate the behavior and transpiration variability of the growing trees.

6.2 Contributions of research

The present research entailed experimental and modelling elements, which included unique components. Together, both parts provided novel findings on the dynamics of young commercial plantations and water flow along the soil-plant-atmosphere continuum.

There is ongoing debate regarding the sustainability and management practices of commercial

plantations in Australia. Therefore, the present research produced useful findings for future policies and licensing procedures. Some specific contributions are described below.

1. **Unique dataset of water and carbon fluxes in young plantation trees in the first 4 years after planting.** Only a few studies have captured the dynamics of water use and carbon assimilation in ecosystems growing rapidly as *E. globulus*. As commercial plantations are extensively planted in Australia and around the world (e.g., Portugal, Brazil, Colombia), this unique dataset might serve as an example for land and water management in different countries.
2. **Quantification of vegetation response to stand growth and climate variability, which can be used to evaluate current management practices.** Measured evapotranspiration at the site did not vary considerably over the years. However, carbon uptake substantially increased over time, with the plantation switching from being an overall carbon source to a carbon sink in approximately 2 years. This challenges the common perception that evapotranspiration rates in plantations are much larger than in pastures already in the first years after establishment.
3. **FETCH3 was developed to simulate water fluxes through the soil, roots, and stem xylem.** This was achieved by restructuring the coupling between these three components of the system when lumping the processes into a single, continuous vertical dimension. The full-coupling between soil, roots, and stem xylem guarantees the continuity of the water fluxes between these three components. The numerical formulation of FETCH3 was verified against exact solutions of simplified expressions of the equations, and the model performance was evaluated against observations of sap flux data collected during five months from a case study.

6.3 Practical Implications

Understanding the trade-offs between water use and carbon assimilation in commercial plantations is important given the economic and ecological impacts caused by plantation establishment and expansion (Saadaoui et al., 2017; Tomé et al., 2021). Therefore, continued cultivation of large scale commercial plantations requires the application of efficient management practices (Stape et al., 2004; White et al., 2010, 2014).

Because most of Australia's commercial plantation trees are established in former agricultural lands (Downham and Gavran, 2020; White et al., 2010), there is a concern that plantation trees may alter the catchment water balance through higher evapotranspiration rates than the former vegetation (Adelana et al., 2014; Dresel et al., 2018). Catchment studies have tried to compare contrasting land uses under the same climate characteristics. Most of these studies focused

on the quantification of evapotranspiration and hydrologic differences between these two land uses. Results from these studies are not definitive, with experimental and modelling studies documenting streamflow reduction with afforestation (Adelana et al., 2014; Azarnivand et al., 2020; Brown et al., 2005) and other studies not finding significant alterations of streamflow (Brown et al., 2015). Some studies reported a decline in the water-table levels, possibly suggesting that plantation trees are consuming more water, through a deeper root system, when compared to pastures (Dean et al., 2016; Dresel et al., 2018).

Large annual transpiration rates often exceeding annual precipitation were observed by Benyon et al. (2006) and Benyon and Doody (2015) across several plantations in the Green Triangle, across South Australia and Victoria. Transpiration rates were especially high where the water table was up to about 6 m from the surface. These observations were used to delineate regulations for commercial plantation in South Australia, where simple water allocation models are being applied in order to represent hydrological consequences of plantation establishments (Greenwood, 2013). Accordingly, *E. globulus* trees are assumed to reach canopy closure after 3 years with evapotranspiration rates increasing in time, thus reducing groundwater recharge, which is estimated to stop completely after 3 years (Figure 2.2). These assumptions were not satisfied in the plantation of the present study, where evapotranspiration rates only slightly increased as the trees grew towards canopy closure. This was caused by the contribution of the understory vegetation to the ET, which was more prominent when the trees were young with a sparse canopy, and gradually decreased and was replaced by tree transpiration. Conversely, the gain in carbon assimilation increased dramatically in the first 2 years after tree establishment, with a rapid increase in water use efficiency.

The results from our study show that local conditions are important in determining the water use of a plantation and that, in some cases, the increase in water consumption might be outweighed by the large gain in carbon assimilation.

6.4 Limitations and future research

6.4.1 Experimental work

The measurements represent a valuable dataset, given the lack of data from growing ecosystem, as discussed in Chapter 2. Limitations to the experimental work are related to the difficulties in measuring important variables such as LAI, soil properties, and interception of rainfall, which certainly would provide more insights on the behavior and productivity of plantations. Part of this limitation was overcome by using allometric equations developed for *E. globulus* trees. Considering that blue gum trees are extensively planted, these type of equations are broadly used in the forestry field. The limited access to the study site also represented

a limitation, especially during the lockdown periods the state of Victoria underwent in 2020 and 2021. This culminated in data being lost due to equipment malfunction during late 2020 and early 2021.

The results of this project highlighted the structural and physiological differences between young and mature trees, when compared to previous studies on mature and well-established forests (Benyon et al., 2009; Benyon and Doody, 2015; Benyon et al., 2006; Pereira et al., 1986). To the global scale, these differences emphasize the need for extensive and continuous research on the ecosystem carbon and water fluxes, as pointed out by several studies (Baldocchi et al., 2021; Cleverly et al., 2020; White et al., 2021). For example, in a recent study, Wardlaw (2022) emphasised the need for ongoing long-term data to understand resilience and predict future trends of terrestrial carbon and water cycle in response to future changing climatic and environmental conditions. In addition, by analysing a comprehensive set of ecosystem functions across a variety of biomes located in different climate zones, Migliavacca et al. (2021) showed that most variability between ecosystem functions is captured by ecosystem productivity, which is mainly explained by vegetation structure.

Therefore, the demand for long-term ecosystem data from a large range of vegetation structures underline the need to monitor a diversity of sites that include variable age, climate, and species. The resultant data sets will provide more accurate estimations of the carbon budget, ecosystem impacts, and forest productivity, which can create the basis for robust management practices and predictions of global ecosystem efficiency.

6.4.2 FETCH3

From a modeling perspective, FETCH3, as the majority of physically-based models, simplifies highly-dynamic processes in order to allow them to be described by mathematical equations. Limitations related to data availability also lead to more simplifications into the model. For example, LAI and height were kept constant even when simulating young trees, which likely impacted the results of the simulations.

The optimization scheme applied, PSO, could be further developed to include more parameters and optimization functions. However, the inclusion of more parameters may not improve the model results since it could over-fit the dataset and add unnecessary complexity to the model. A balance between parametrization and simplicity should be evaluated, also considering that most of the empirical parameters may not always have physical meaning. Currently, there are efforts to calibrate FETCH3 against evapotranspiration data from the AmeriFlux network, using a different calibration approach. These new studies might provide further insights on the calibration and parametrization of FETCH3, certainly benefiting the model outputs. Additional efforts into the calibration and enhancement of FETCH3 might improve model performance during periods of high variable transpiration, such as the case for the dry period at Digby Plant-

ation.

Future developments into FETCH3 should also focus in improving model processes. A good option would be the implementation of a more comprehensive transpiration formulation, as the Ball et al. (1987), Leuning (1990), and Leuning (1995), and stomata conductance optimization as Qiu and Katul (2020) and Liu et al. (2020). These approaches mechanistically describe the stomatal behavior and reproduce the hydraulic dynamics in the leaf by assuming that stomata conductance is proportional to carbon assimilation. This can lead to a better trait representation and estimations of transpiration variability.

Another valuable future contribution into FETCH3 would be the inclusion of tree growth into the solution of the equations, including dynamic xylem area, root depth, root density, and tree height. Even though FETCH3 algorithm allows to update parameters in time and space, changing xylem area and other structural tree parameters during the simulation would create an increment of water unaccounted for in the water and mass balance. This would create numerical instabilities that could ultimately add errors in the numerical scheme of the model. Further studies are required to estimate those errors and identify the best approach to account for xylem area variability and growth. Tree growth is an important factor that contributes to tree transpiration and tree-trait representation, and it would allow a more realistic modelling of plantation structure and development. However, developing a tree growth module into FETCH3 might add more complexity in the solution of the equations, so future research might also focus on a balance between model complexity and performance.

Future directions for FETCH3 could also include the addition of coexistence of species. This would provide the model with more realism, considering that even in monocultures, the presence of understory vegetation, for example, can impact the water balance and increase ecosystem water use. This would likely improve simulations of young and developing trees, such as the plantation monitored in this project. Lastly, the modelling of soil temperature, and the production of CO₂ from soil microorganisms and plant roots could provide valuable insights in the behavior and trait-based representation of trees and also improve the description of the key mechanisms regulating root water uptake.

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