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Rémi Vezy

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THÈSE PRÉSENTÉE PAR

**Rémi VEZY**

POUR OBTENIR LE GRADE DE

**DOCTEUR DE**

**L'UNIVERSITÉ DE BORDEAUX**

ÉCOLE DOCTORALE SCIENCE DE L'ENVIRONNEMENT

SPÉCIALITÉ PHYSIQUE DE L'ENVIRONNEMENT



**SIMULATION DE PRATIQUES DE GESTION  
ALTERNATIVES POUR L'ADAPTATION DES  
PLANTATIONS PERENNES AUX  
CHANGEMENTS GLOBAUX**

**Soutenue le 19 décembre 2017**

Membres du jury :

**M. Denis LOUSTAU**

**M. Gueric LE MAIRE**

M. Thierry FOURCAUD

M. Christian DUPRAZ

M. Hendrik DAVI

Mme Andrée TUZET

M. Bruno RAPIDEL

M. Olivier ROUPSARD

UMR ISPA, INRA Villenave d'Ornon

UMR ECO&SOLS, CIRAD Montpellier

UMR AMAP, CIRAD Montpellier

UMR SYSTEM, INRA Montpellier

URFM, INRA Avignon

UMR ECOSYS, INRA Thiverval-Grignon

UMR SYSTEM, CIRAD Montpellier

UMR ECO&SOLS, CIRAD Dakar

Directeur de thèse

Co-Directeur

Rapporteur

Rapporteur

Rapporteur

Examineur

Examineur

Examineur









## Résumé :

Les effets des changements climatiques sur les systèmes agronomiques sont encore très incertains. Par conséquent, il existe un besoin croissant d'informations pour mieux prédire les impacts futurs des changements climatiques sur les cultures pérennes et les forêts, ainsi que pour concevoir de nouvelles pratiques agricoles et sylvicoles pour faire face à ces changements (Brisson et al., 2010). Ces changements ont des effets combinés complexes sur les bilans d'énergie, hydriques et de carbone des écosystèmes, et peuvent donc affecter la production des agroécosystèmes (Way et al., 2015).

Les modèles basés sur les processus (PBM) sont généralement bien adaptés pour relever ces défis. Ils appliquent notre compréhension des processus physiques et écophysologiques fondamentaux pour simuler physiquement le système (Bohn et al., 2014). Ils peuvent être utilisés pour estimer les flux et les stocks d'énergie, d'eau et de carbone dans l'écosystème, en fonction des caractéristiques du climat, du sol et des plantes.

La croissance du café et la production de fruits sont particulièrement sensibles aux températures élevées et à la disponibilité de l'eau, et des études antérieures prédisent souvent une perte conséquente de production ou une réduction des aires potentielle de culture. Néanmoins, l'ombrage fourni dans les systèmes agroforestiers pourrait atténuer les effets des changements climatiques selon différentes options de gestion. Ainsi, au cours de cette thèse, nous avons d'abord mis à jour un PBM 3D (MAESPA) pour tenir compte de la température et de la pression de vapeur dans la canopée, puis l'avons validé sur deux écosystèmes : une plantation d'Eucalyptus au Brésil et une plantation de *Coffea arabica* au Costa Rica. Nous avons ensuite utilisé MAESPA pour créer des métamodèles qui ont été intégrés à un nouveau modèle de croissance et de rendement développé pour évaluer la réponse du caféier au changement climatique et les solutions possibles offertes par la gestion agroforestière pour atténuer ces effets. Nous avons modélisé plusieurs options de gestion des systèmes d'agroforesterie de café, parmi lesquels la densité et les essences d'arbres d'ombrage afin d'estimer leur adéquation ainsi que leur apport en services écosystémiques sous changements climatiques. Une comparaison entre les scénarios de gestion a ensuite été proposée en comparant la température de la canopée, le rendement des caféiers, le bilan carbone et l'utilisation de l'eau pour chaque cycle de croissance du café passé et futur. Le modèle de croissance prédit une augmentation de la productivité primaire des caféiers avec l'augmentation de la concentration en CO<sub>2</sub> atmosphérique, mais une réduction du rendement de grains due à une réduction du nombre de fleurs d'ici l'horizon 2100. Le modèle prédit un effet positif de l'ombrage sur les rendements avec l'augmentation des températures, jusqu'à +20.9% comparativement à la culture sous plein soleil sous RCP8.5. Cependant, l'ombrage ne permet pas de maintenir les rendements aux niveaux actuels dans le modèle, quelle que soit la gestion utilisée.

## Résumé vulgarisé :

Dans le cadre de cette thèse, nous avons utilisé deux modèles mathématiques complémentaires pour simuler le comportement futur des plantations de café sous conditions actuelles ainsi que sous changements climatiques (1979 -2100). Nous avons étudié leurs bilans de carbone, d'eau et d'énergie pour mieux comprendre et prévoir les effets des changements sur la production de café. Comparativement à une plantation en plein soleil, l'ajout d'arbres d'ombrage au dessus des caféiers pourrait permettre d'augmenter les rendements lorsque la température augmente. Cependant, les rendements en grain de caféiers à l'horizon 2100 sont prédits inférieurs aux rendements actuels quelle que soit l'espèce d'arbres d'ombrage ou sa gestion.

**Mots-clés : MAESPA, écophysologie, café, eucalyptus, agroforesterie, modélisation, changements climatiques**

Laboratoires d'accueil : UMR ISPA INRA, Villenave D'ornon / UMR ECO&SOLS CIRAD, Montpellier



## **Summary:**

Many agronomic systems could be at risk considering the short-term climate changes, but several effects and interactions are still uncertain. Therefore, there is an increasing need for information to better predict future climate change impacts on perennial crops and forests and to design new agricultural and silvicultural practices to cope with these changes (Brisson et al., 2010). All those changes lead to complex combinations of effects on the water and carbon balances of ecosystems, and can thus, potentially, affect agro-ecosystem production (Way et al., 2015).

Process-based models (PBMs) are generally well suited to address these challenges. PBMs apply our understanding of fundamental physical and ecophysiological processes to simulate the system mechanistically (Bohn et al., 2014). They can be used to estimate fluxes and stocks of energy, water, and carbon in the ecosystem, as a function of climate, soil, and plant characteristics.

Coffee growth and fruit production are particularly sensitive to high temperatures and water availability, and previous studies often predicts future huge losses of production or area cover. Nevertheless, shade provided in agroforestry systems could mitigate the effects of climate changes under different management options. Hence, during this thesis, we first updated a 3D PBM (MAESPA) to account for temperature and vapor pressure within the canopy, and tested it on two ecosystems, a Eucalyptus plantation in Brazil, and *Coffea arabica* plantation in Costa Rica. Then, we used MAESPA to make metamodels that were integrated on a new dynamic crop model that we developed to assess the *Coffea* response to climate change, and the possible solutions offered by different agroforestry management to mitigate these effects. Consequently, we modelled several management options of coffee agroforestry systems, e.g. shade tree density and species to estimate their suitability and provision of ecosystem services under predicted future climate changes. A rating between management scenarios was then proposed by comparing canopy temperature, coffee and timber yield, carbon balance and water use of past and future coffee growth cycles, under two contrasted future climatic scenarios (RCP 4.5 and 8.5). The dynamic crop model predicts an increased coffee primary productivity thanks to the increased atmospheric CO<sub>2</sub> concentration, but a decreased coffee yield because less flowers were initiated per coffee plants by 2100. The model predicts a positive shade effect on coffee yield, especially under high mean annual temperatures, up to +20.9% yield compared to full sun plantation under RCP8.5. However, the positive effect of shade couldn't help sustaining current yields, whatever the shade tree species or management.

## **Popularized summary:**

In this thesis, we used two complementary mathematical models to simulate the future behavior of coffee plantations under climate change (1979 - 2100). We studied their carbon, water, and energy balances to better understand and predict the effects of these changes on coffee production. The addition of shade trees above the coffee layer lead to higher yield compared to full sun management under increased temperature. However, coffee yield was predicted to decrease compared to current levels by 2100, whatever the shade tree species or management.

**Keywords:** MAESPA, ecophysiology, coffee, eucalyptus, agroforestry, modelling, climate change



## Remerciements

*"Nos esse quasi nanos, gigantium humeris insidentes, ut possimus plura eis et remotiora videre, non utique proprii visus acumine, aut eminentia corporis, sed quia in altum subvenimur et extollimur magnitudine gigantea"*. Cette phrase est empruntée à Bernard de Chartres, et ce traduit par "nous sommes comme des nains assis sur des épaules de géants. Si nous voyons plus de choses et plus lointaines qu'eux, ce n'est pas à cause de la perspicacité de notre vue, ni de notre grandeur, c'est parce que nous sommes élevés par eux".

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# Chapitre 1. Introduction

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## 1.1. Les changements climatiques

### 1.1.1. Modélisation du climat et prévisions à long terme

Le climat a longtemps conditionné le développement de l'humanité, et a parfois été le facteur dominant de changements sociétaux, voire d'extinction de civilisations (Dearing, 2006). Comprendre, prévoir et s'adapter au climat changeant est donc une obligation pour garantir la pérennité de la sécurité alimentaire malgré l'augmentation de la population.

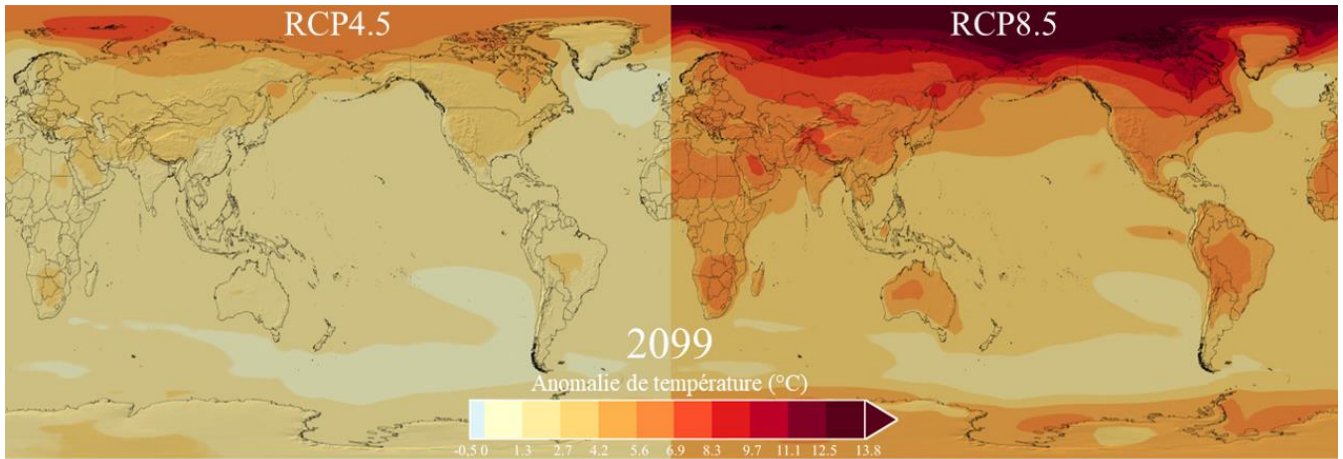
Le climat décrit la tendance météorologique d'une région sur une période donnée. La météorologie est l'étude des phénomènes atmosphériques qui vise à mesurer, comprendre, et prédire les conditions atmosphériques comme la température, la pression et l'humidité relative, mais aussi la formation des nuages, des orages, de la neige, de la grêle, des vents moyens et des rafales, ainsi que des précipitations. Il s'agit d'une science multidisciplinaire car les processus décrivant l'état de l'atmosphère peuvent eux-mêmes dépendre de l'état d'autres systèmes, dont les océans, les sols, la végétation, les surfaces enneigées ou encore les milieux urbains. Elle est le plus souvent associée à des périodes d'études relativement courtes, allant de la demi-heure à la dizaine de jours. La climatologie quant à elle est une représentation statistique des conditions météorologiques moyennes pendant une période déterminée.

Prévoir les conditions météorologiques requiert des modèles complexes, mais surtout des données d'initialisation précises et en grand nombre car le système atmosphérique est chaotique, c'est-à-dire qu'une erreur très fine sur les paramètres initiaux peut donner des prévisions très différentes (Lorenz, 1963). La durée limite au-delà de laquelle la prévision d'un modèle numérique est considérée comme non fiable est appelée la prévisibilité. Les modèles météorologiques européens ont en général une prévisibilité d'environ trois jours, mais il existe plusieurs moyens de la dépasser (*e.g.* plus d'observations, prévisions d'ensemble, approche multi-modèle) pour arriver à une prévisibilité de 7 à 10 jours. Les modèles météorologiques ne sont donc pas adaptés pour des prévisions à long terme, qui seront donc effectuées par des modèles de tendances, ou autrement dit des modèles climatiques.

Il existe de nombreux types de modèles climatiques, utilisant des méthodes de calculs différentes, ainsi que des échelles spatiales et temporelles différentes. Les modèles climatiques les plus élaborés sont les modèles de circulation générale couplé océan-atmosphère (AOGCM), ainsi que leurs dérivés les ESMs "Earth System Model", qui ajoutent les cycles biogéochimiques à l'échelle de la Terre pour compléter le cycle du carbone. Le projet d'inter-comparaison des modèles couplés (CMIP) sert à répertorier, tester et comparer les nombreux modèles climatiques existants dans un même cadre défini. Les derniers tests du groupe en date (CMIP6) ont répertorié 33 groupes de recherches provenant du monde entier, ainsi que plus de 70 modèles testés (Jones et al., 2016; Taylor et al., 2012). Le projet propose quatre grands scénarios de forçage radiatif (RCP) qui représentent la différence entre l'énergie reçue (en  $W m^{-2}$ ) et l'énergie réémise par la Terre en 2100 comparativement à 1750 (Moss et al., 2010). Ces scénarios radiatifs sont eux-mêmes basés sur des scénarios d'émissions de gaz à effets de serre, et reflètent leur effet sur l'équilibre énergétique de la Terre. Ils correspondent chacun à une trajectoire plausible de conditions climatiques futures en fonction des émissions

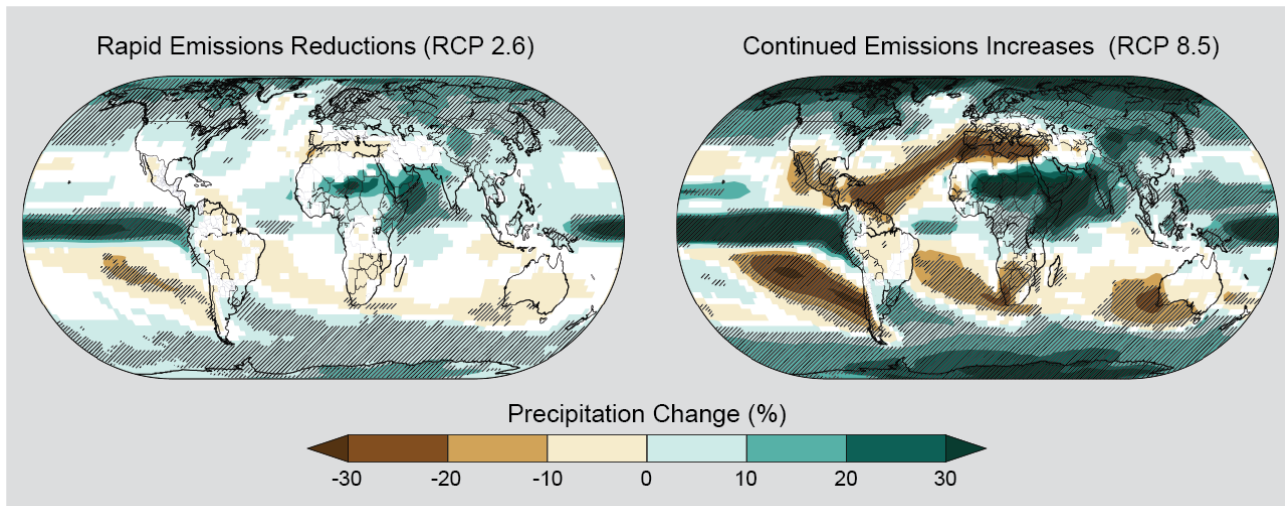


anthropiques de CO<sub>2</sub> et autres gaz à effets de serre actuelles et futures, partant de la plus modérée dans laquelle l'humanité mettrait en place des politiques fortes en faveur de l'atténuation de ses émissions (RCP2.6, 10<sup>e</sup> percentile des scénarios avec atténuation) jusqu'à la plus soutenue dans laquelle l'humanité maintiendrait ses émissions au niveau actuel (RCP8.5, 90<sup>e</sup> percentile des scénarios sans atténuation).



**Figure 1. Prédiction des anomalies de température à la surface du globe pour 2099. Les données proviennent d'une moyenne des prédictions des modèles du CMIP5 (Coupled Model Intercomparison Project Phase 5). Source : NASA Center for Climate Simulation/Scientific Visualization Studio.**

Les changements climatiques ont probablement déjà contribué à un réchauffement des températures de surface de 0.5 à 1.3°C sur la période 1951-2010, et les modèles prédisent en moyenne une augmentation de 1.8°C (intervalle de confiance 5-95% : 1.1°C et 2.6°C) sous RCP4.5, et 3.7°C (2.6 à 4.8°C) sous RCP8.5 en 2100 comparativement à la période de référence 1986–2005. Cependant, l'augmentation des températures moyennes de surface sera probablement très hétérogène au travers du globe (Figure 1), avec des augmentations de températures plus élevées aux pôles que partout ailleurs et plus élevées sur les surfaces continentales que sur celle des océans, ainsi que relativement plus élevées en régions tropicales et subtropicales à court-terme (Pachauri et al., 2014). Les précipitations seront probablement aussi très impactées par les changements climatiques, avec en général plus de précipitations dans les régions pluvieuses, et moins de précipitations dans les régions déjà sèches (Liu et al., 2012). Cependant, les modèles donnent parfois des prédictions incohérentes entre eux, principalement à cause des processus régionaux implémentés ou non (Figure 2).



**Figure 2. Changements des précipitations projetés pour 2100. Variation des précipitations annuelles moyennes projetées pour la période 2071-2099 en comparaison avec la période 1970-1999 pour RCP 2.6 et 8.5. Les zones hachurées indiquent que les changements prévus sont significatifs et cohérents entre les modèles. Les zones blanches indiquent que les changements ne devraient pas être plus importants que ce que l'on pourrait attendre de la variabilité naturelle. Source : NOAA NCDC / CICS-NC.**

### 1.1.2. Effets du climat sur les cultures

Puisque chaque plante dispose d'un optimum environnemental, son aire de répartition est intimement liée au climat qui l'entoure (Thuiller et al., 2004; Ramankutty et al., 2002). De plus, l'intrication remarquable des effets environnementaux sur les cultures en fait un système complexe à appréhender. Ainsi, la lumière visible permet la photosynthèse, qui transforme le CO<sub>2</sub> atmosphérique capté par la plante en sucres, la température influe sur la production nette de carbone des plantes par son effet sur la photosynthèse et sur la respiration, et agit conjointement avec l'humidité de l'air sur la transpiration de la plante par l'effet de demande évaporative. La plante contrôle l'ouverture de ses stomates pour réguler sa transpiration et éviter la dessiccation, ce qui impacte aussi la photosynthèse, car les stomates sont les organes d'échange entre la plante et l'atmosphère pour l'eau, mais aussi pour le CO<sub>2</sub>. La transpiration joue à son tour sur la température des feuilles, mais dépend aussi de l'énergie reçue et de l'état hydrique de la plante, qui dépend à son tour de celui du sol, qui est lui-même contrôlé par les précipitations. Le vent quant à lui va favoriser les échanges gazeux entre les feuilles de la plante et l'atmosphère en réduisant la couche limite à leur surface (Jones, 2013). A l'échelle annuelle, certaines plantes ont aussi développé une dépendance à des événements climatiques particuliers pour leur phénologie végétative et reproductive. Par exemple les céréales d'hiver ont besoin de conditions hivernales (vernalisation) pour passer du cycle de développement végétatif au cycle reproductif (Chouard, 1960), la vigne a une floraison plus synchronisée après un passage au froid (Rivals, 1963), et le caféier a lui aussi une floraison plus synchronisée, mais après une courte période de sécheresse suivie d'un événement de pluie pour déclencher la sortie de dormance de ses bourgeons floraux (Cannell, 1985). Enfin, le climat peut aussi jouer sur la présence de ravageurs et de parasites, qui ont eux aussi leur propre optimum environnemental.

### 1.1.3. Prévisions des productions agricoles futures

Si les émissions des gaz à effet de serre maintiennent leur augmentation actuelle, les changements climatiques risquent d'amplifier la vulnérabilité des systèmes agricoles, et ainsi réduire les productions dans certaines régions du monde (Figure 3). Cependant, ces dernières pourraient tout aussi bien augmenter dans d'autres régions. Il est en effet difficile de prévoir leurs conséquences car la direction et l'amplitude des changements vont dépendre de nombreux facteurs (Zhang et al., 2017). Ainsi, l'augmentation de la concentration atmosphérique du CO<sub>2</sub> pourrait éventuellement augmenter la productivité des plantes, ainsi que leur efficacité d'utilisation de l'eau (Hatfield et al., 2011). Cependant, Ellsworth et al. (2017) ont montré qu'une augmentation du CO<sub>2</sub> ne s'accompagnait pas nécessairement d'une augmentation de la production lorsque la culture est limitée par d'autres facteurs comme le phosphore, ce qui est le cas de beaucoup de sols tropicaux. L'augmentation des températures et la modification du régime des précipitations auraient quant à elles un effet négatif sur la production de céréales, notamment à cause du stress engendré par des pics de chaleurs durant le remplissage des grains, ainsi que par les sécheresses (Ainsworth and Ort, 2010), et les cultures intensives seraient notamment particulièrement touchées par ce phénomène (Brisson et al., 2010). Par exemple, Barros et al. (2014) montrent que les premières pertes de productions risquent de se produire à partir de 2020 dans les zones semi-arides en Afrique (IPCC AR5 WG2 [22.3.4]), puis vont progressivement apparaître en Amérique centrale et du Sud, au Mexique, en Asie (IPCC AR5 WG2 [24.4.4,25.2,25.7,27.3.4]), et en Europe du Sud (Olesen and Bindi, 2002). Les changements climatiques pourraient aussi favoriser l'apparition de pathogènes et d'insectes dans certaines régions, ce qui réduirait encore les productions (Hatfield et al., 2011;Roos et al., 2011;Newbery et al., 2016). Toutefois, les changements climatiques pourraient avoir un effet positif sur les productions céréalières dans certains pays du Nord par l'expansion des terres cultivables, l'introduction de nouvelles variétés jusque-là non adaptées aux conditions climatiques de ces zones, et l'augmentation du rendement grâce notamment à l'augmentation de la concentration en CO<sub>2</sub> atmosphérique. Par conséquent, il est difficile de donner une réponse unique quant aux effets des changements climatiques sur les productions agricoles à l'échelle mondiale car les multiples interactions et rétroactions possibles entre tous les processus en jeu rend leur prévision difficile.

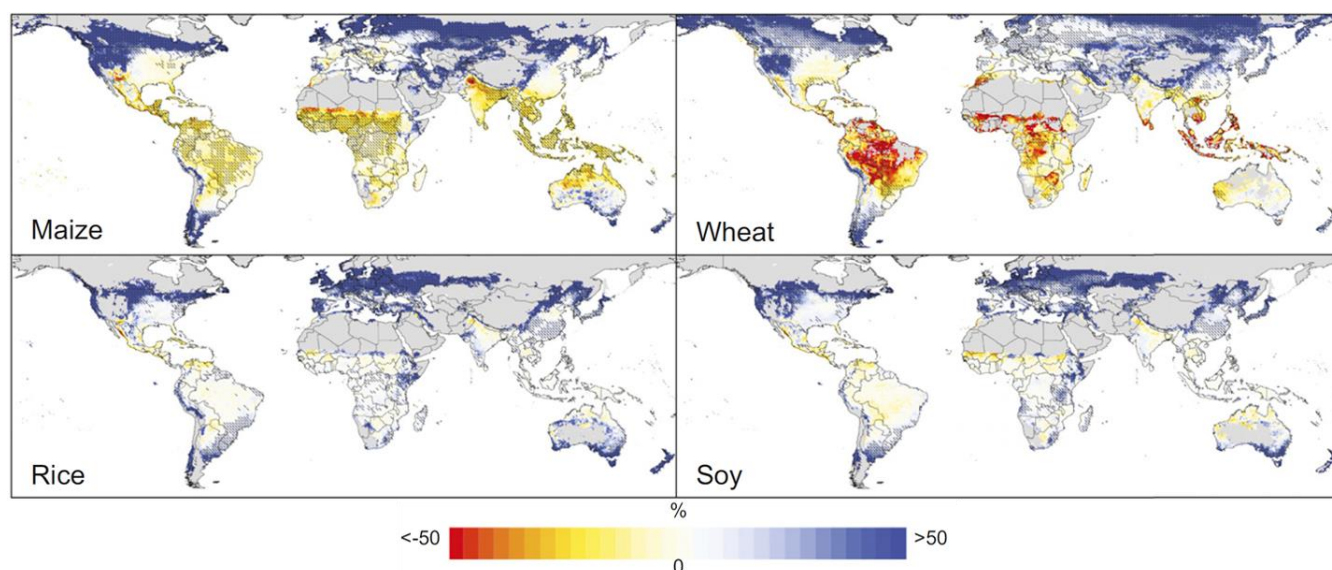


Figure 3. Prédiction des changements médians de productions (%) avec effet du CO<sub>2</sub> pour la période 2070–2099, en comparaison avec la période de base 1980–2010 pour RCP8.5. Source: Rosenzweig et al. (2014). Maize= Maïs, Wheat= blé, Rice= riz et Soy= soja.

## 1.2. L'adaptation des plantations aux changements climatiques

### 1.2.1. Les principales solutions d'adaptation actuelles

L'adaptation des cultures potentiellement négativement impactées par les changements climatiques est un grand défi pour l'homme, car les solutions sont difficiles à appréhender. En effet, il ne s'agit non pas d'adapter les cultures à des conditions existantes, mais bien à un environnement absent des conditions actuelles, et donc difficilement testable par expérimentation. Il est donc primordial de trouver des outils qui nous permettent d'adapter nos systèmes de production aux conditions futures afin de maintenir des productions suffisantes, tout en favorisant leur résilience grâce à un développement de systèmes durables. Plusieurs solutions peuvent être proposées pour adapter les cultures aux changements, parmi lesquelles on peut citer :

- La modification du calendrier de gestion des cultures annuelles, avec par exemple un semis précoce (Kalra et al., 2008) ;
- Le changement de la variété ou de l'espèce cultivée pour une autre plus résistante aux nouvelles conditions abiotiques (pic de chaleurs, sécheresse...) comme biotiques (ravageurs, parasites...), ce qui peut impliquer de nouvelles variétés issues de croisements génétiques (Smit and Skinner, 2002) ;
- L'utilisation intensive de technologies de gestion de l'eau, comme l'irrigation ou la rétention d'eau par les résidus de cultures (Ramankutty et al., 2002;Howden et al., 2007;Hatfield et al., 2011) ;
- L'utilisation de techniques agroécologiques comme la diversification des productions ou l'agroforesterie pour augmenter leur résilience grâce à la facilitation entre espèces (Trnka et al., 2011;Rötter et al., 2013;Altieri and Nicholls, 2017) ;
- L'intégration de nouvelles technologies (Smit and Skinner, 2002) comme les données satellite pour la gestion de l'irrigation (Battude et al., 2017;Veysi et al., 2017), l'identification précoce des ravageurs (Mall et al., 2016;Groeneveld, 2017) ou de la demande en nutriments (Fitzgerald et al., 2010;Huang et

al., 2017); l'utilisation de systèmes de prévisions météorologiques localisés pour la prévention précoce des risques (Wu et al., 2016); ou encore de la robotique pour l'aide à la gestion.

Il est à noter que l'efficacité de ces adaptations dépendra des futures conditions climatiques de chaque région et du type de culture, mais aussi de la disponibilité en ressources et en infrastructures mises en place par les gouvernements (Olesen and Bindi, 2002). L'approche que proposent certaines institutions comme la FAO (Asfaw and Lipper, 2016) ou la banque mondiale (Klytchnikova et al., 2015) est de transformer l'agriculture actuelle en agriculture intelligente face au climat, aussi appelée Climate-Smart Agriculture en anglais (CSA). La CSA est une stratégie qui viserait à augmenter de façon durable la productivité agricole pour atteindre des niveaux de sécurité alimentaire désirables en renforçant la résilience et la capacité d'adaptation des systèmes agricoles, tout en réduisant les émissions de gaz à effet de serres, ou même en séquestrant du carbone (Lipper et al., 2014). Divers projets pilotes ont identifié des moyens pratiques comme la diminution du labour pour réduire le déstockage du carbone, l'arrêt de la culture sur brûlis, l'utilisation de l'agroforesterie, les systèmes sylvopastoraux, la culture intercalée, l'ajout de cultures ciblées entre les rotations (Klytchnikova et al., 2015).

### **1.2.2. Le cas particulier des plantations pérennes**

Les cultures pérennes représentent un enjeu social et économique majeur. Le secteur forestier emploie par exemple directement 13.2 millions de personnes dans le monde à lui seul (0.4% des actifs du monde) principalement en Asie, en Océanie et en Europe. De plus, la production mondiale issue du secteur forestier (bois rond, sciage, panneaux et pâte à papier) était de 600 milliards de dollars US en 2011 dans le monde, soit 0.9% du produit intérieur brut mondial, sans compter 123.6 Md\$ provenant de produits dérivés tels que la production d'énergie, la construction ou les plantes médicinales (FAO, 2014). Toutefois, les plantations pérennes seront particulièrement touchées par les changements climatiques, car une parcelle plantée aujourd'hui devra pouvoir faire face à toutes les conditions climatiques qu'elle sera sujette à rencontrer durant sa rotation, de quelques années à plusieurs décennies. De plus, elles sont plus difficiles à adapter par la sélection génétique que les plantations annuelles car leurs cycles de croissance sont plus longs, donc l'expression des traits désirés peut prendre plusieurs décennies.

Cependant, les plantations pérennes ont un fort potentiel d'adaptation par la gestion, qui va elle-même surtout dépendre des changements qui vont affecter la culture d'intérêt. Par conséquent, si les régimes de pluviométries sont modifiés vers une tendance à plus de sécheresse, l'adaptation de la plantation peut se faire grâce à une réduction de la densité à la plantation, à une réduction de la fertilisation pour limiter l'indice de surface foliaire (LAI) (Battie-Laclau et al., 2014), à une mise en place d'éclaircies pendant la rotation (White et al., 2009) ou à une réduction des temps de cycle de rotation pour éviter les stades de croissance qui ont une moins bonne efficacité de l'utilisation de l'eau (Christina et al., submitted). On peut aussi mélanger différentes espèces pour augmenter la résilience du système (Germon et al., 2017), modifier l'aménagement du territoire pour prévenir les dommages liés aux feux, aux tempêtes ou aux ravageurs (Howden et al., 2007), ou ajouter des arbres d'ombrages pour tamponner les températures extrêmes (Sida et al., 2018). Dans tous les cas, étant

donné que l'ampleur des changements climatiques est très incertaine, il semblerait que la meilleure stratégie à adopter soit celle de l'augmentation de la résistance et de la résilience des systèmes (Lin, 2011).

### 1.2.3. Le cas particulier de l'agroforesterie

Les systèmes agroforestiers (SAF, AFS en anglais) sont un type de culture stratifié, dans lequel une plante basse est cultivée en association avec des arbres. Il existe de nombreux systèmes agroforestiers qui diffèrent par les espèces utilisées et leur gestion, mais toujours conçus de manière à ce que la concurrence entre espèces soit réduite pour favoriser l'acquisition complémentaire des ressources qui ne seraient pas pleinement exploitées autrement (Cannell et al., 1996). Les AFS ont de nombreux avantages. Par exemple, l'association de *Faidherbia albida* avec du blé a montré une amélioration du remplissage des grains de blé et une augmentation de la productivité grâce notamment à l'effet tampon des arbres d'ombrage sur les conditions climatiques extrêmes éthiopiennes (Sida et al., 2018), tout en réduisant la compétition pour la lumière et l'eau grâce à la phénologie opposée entre *F.albida* et la plupart des cultures et au caractère phréatophyte de *Faidherbia* (Roupsard et al., 1999). Il a aussi été mesuré un renforcement du stockage de carbone dans des associations noyers-blé dur (Chenu et al., 2015;Cardinael et al., 2015), une réduction de la lixiviation de nitrates (Nair et al., 2007), une augmentation de l'exploration racinaire dans une association *Eucalyptus grandis* et *Acacia mangium* (Germon et al., 2017), des effets positifs directs sur la productivité et la fertilité du sol (Ong and Kho, 2015), la rétention d'eau (Verchot et al., 2007), la biodiversité (De Beenhouwer et al., 2013), la réduction du vent (Luedeling et al., 2016), et dans certaines conditions une réduction des ravageurs par l'augmentation de leur ennemis naturels (Lin, 2011). L'agroforesterie a donc le potentiel de limiter les effets des changements climatiques et d'adapter les productions (Lin, 2011;Luedeling et al., 2014).

Toutefois, les AFS ont tout de même certains inconvénients. En effet, l'ajout d'arbres diminue la lumière transmise à la culture, ce qui peut entraîner une diminution de sa productivité. Il peut aussi y avoir des compétitions pour l'eau et les nutriments si la gestion est mal assurée ou que le sol et/ou les choix d'espèces en association ne se prête pas à une claire séparation verticale des systèmes racinaires de l'arbre et des cultures intercalaires (Padovan et al., 2015;Abdulai et al., 2017). Il existe néanmoins des pratiques pour limiter la compétition en surface, comme le cerclage des racines de l'arbre. Ces effets de compétition peuvent être un frein à l'adoption de l'agroforesterie, cependant la baisse de production de la culture de sous-bois est très souvent compensée voire dépassée par la production des arbres, que ce soit en fruits, en bois ou plus indirectement en apports azotés (Verchot et al., 2007). Ce concept est d'ailleurs caractérisé par le LER (Land-equivalent ratio), qui représente le gain de productivité en comparant la culture AFS avec une parcelle de même surface subdivisée en autant de sous-placettes monospécifiques que d'espèces contenues dans l'AFS (Malézieux et al., 2009). Un LER supérieur à 1 signifiera donc que l'AFS aura une production nette supérieure à la somme de ces homologues monospécifiques, ce qui peut être expliqué par le fait que les AFS ont tendance à avoir une meilleure utilisation des ressources (Dupraz and Liagre, 2008).



Les avantages considérables amenés par les AFS, et tout particulièrement les effets sur le microclimat de la culture (Lin, 2007;Siles et al., 2010;Sida et al., 2018), en font une gestion à fort potentiel pour adapter les cultures aux changements climatiques (Nair, 2012). De plus, leur adoption progressive est attendue grâce notamment à une meilleure dissémination des informations à leur sujet grâce à l'apparition d'organismes spécialisés comme l'association française d'agroforesterie ou le world agroforestry centre (ICRAF), des incitations financières via des labélisations (*e.g.* Rainforest Alliance) ou paiements pour services écosystémiques (*e.g.* l'ONG GRET), ainsi qu'à des planifications politiques tels que le plan national de développement pour l'agroforesterie en France, ou la politique agricole commune (PAC) en Europe.

### **1.3. La modélisation des cultures pérennes.**

#### **1.3.1. L'apport de la modélisation**

Les expérimentations en laboratoire et sur le terrain sont sans nul doute les meilleurs moyens de tester les réponses d'une plante à un facteur. Cependant, les expérimentations sur les cultures pérennes sont souvent coûteuses, mal adaptées pour les expérimentations sous conditions climatiques contrôlées, et le nombre d'itinéraires techniques et/ou de composition spécifique peut vite devenir relativement grand (Porté and Bartelink, 2002). En effet, les expérimentations de laboratoires sont souvent uniquement faites sur de jeunes individus, et ne représentent pas tous les processus réellement à l'œuvre dans une parcelle (enracinement, vent, ensoleillement, interactions...). De plus, bien que les expérimentations de terrain permettent d'étudier certains effets prédits des changements climatiques, comme le manque d'eau grâce à la mise en place d'exclusions de pluies (Christina et al., 2015;Estiarte et al., 2016), ou l'augmentation de la concentration en CO<sub>2</sub> atmosphérique comme dans les projets FACE (Ainsworth and Long, 2005;Duursma and Medlyn, 2012b;DaMatta et al., 2016), elles ne permettent pas pour l'instant d'étudier pleinement les interactions de ses effets en prenant en compte à la fois la sécheresse, l'augmentation de [CO<sub>2</sub>] et l'augmentation des températures. C'est pourquoi sans remplacer l'immense valeur qu'apporte l'expérimentation, la modélisation peut être un bon outil complémentaire pour étudier les plantations pérennes (Palma et al., 2007;Bohn et al., 2014;Norby et al., 2016). En effet, elle permet de résumer et formaliser l'état de l'art des connaissances sur les nombreux processus en jeu, mais aussi de mieux les comprendre en les testant sur des systèmes réels. Ensuite, elle permet de résoudre l'interaction des nombreux processus difficiles à appréhender en peu de temps et d'efforts (Ebi et al., 2016). Cela signifie que les modèles peuvent être un vrai atout pour nous permettre de résumer, appliquer et généraliser nos connaissances dans l'espace (de l'échelle feuille à globale) et dans le temps (passé, présent, futur). Ils pourront donc être utilisés pour anticiper les conséquences des changements climatiques sur les plantations, et prédire les meilleures gestions à mettre en place pour l'adaptation des cultures (Webber et al., 2014). Il n'en reste pas moins qu'un cercle vertueux de la recherche mobilise à la fois l'Observation, l'Expérimentation et la Modélisation et que chaque pilier soutient l'ensemble de la compréhension d'un phénomène donné.

### 1.3.2. Les grands types de modèles

Il existe de nombreux types de modèles applicables aux plantations pérennes, avec des structures et des complexités très différentes liées à des objectifs variés. Pretzsch et al. (2015) relèvent par exemple 54 modèles différents. De nombreuses classifications ont été proposées comme le montrent Porté and Bartelink (2002), cependant trois grandes catégories sont souvent rencontrées (Kimmins, 1990; Fontes et al., 2010): les modèles empiriques (EM), les modèles basés sur des processus (PBM), et les modèles hybrides (HM). Une quatrième catégorie peut aussi y être ajoutée avec les "gap models" (modèles de trouées).

#### *Modèles empiriques (EM)*

Les modèles empiriques sont généralement générés et calibrés à partir de relations descriptives issues d'inventaires (Porté and Bartelink, 2002). Ils sont plutôt utilisés à l'échelle du peuplement, mais certains sont tout de même basés sur des relations à l'échelle de l'arbre (Landsberg et Sands 2010). Ces modèles sont faciles à utiliser car ils nécessitent peu de données explicatives, et donnent de bons résultats en général. Cependant, ils ne peuvent pas être utilisés pour des extrapolations à d'autres systèmes ou à de nouvelles conditions environnementales (Porté and Bartelink, 2002; Kahle, 2008) parce qu'ils reposent sur des relations de corrélations sans décrire complètement le comportement du système (Adams et al., 2013). Néanmoins, les modèles dynamiques d'état-espace ("dynamic state-space") et le développement de modèles empiriques prenant en compte des relations productivité-environnement sont des approches qui ont le potentiel de prendre en compte des changements de conditions environnementales dans la gamme de variabilité (et de corrélations) dans lesquelles ils ont été entraînés (Fontes et al., 2010). Toutefois, tous les modèles empiriques utilisent par définition des mécanismes implicites dérivés de corrélations mais pas de causes, ce qui a tendance à biaiser leurs prédictions dès qu'ils sont appliqués à de nouvelles conditions (Adams et al., 2013). De ce fait, leur simplicité devient un inconvénient lorsque les conditions environnementales changent radicalement (Fontes et al., 2010), faisant des modèles empiriques de mauvais candidats pour la modélisation des plantations pérennes sous changement climatiques, et tout particulièrement pour étudier l'effet de gestions nouvelles.

#### *Modèles basés sur les processus (PBM)*

Contrairement aux modèles empiriques, les PBM utilisent des processus écophysiologiques explicites et fondamentaux comme l'interception de la lumière, la photosynthèse, ou la respiration pour simuler le système de façon physique (Bohn et al., 2014). Ainsi, le système est simulé comme un système hiérarchique (Bugmann et al., 2010), en utilisant un ensemble complexe de sous-modèles en interaction les uns avec les autres. Le modèle est donc capable de décrire les processus qui conduisent à des changements dans l'état de la plante à partir des variables environnementales de forçage (Landsberg and Sands, 2010). Toutefois, tous les PBM finissent par utiliser des descriptions empiriques à un certain point, et il existe toujours un compromis entre la finesse des processus décrits par le modèle et la difficulté pour l'obtention de leurs paramètres.



Ces modèles conviennent particulièrement pour des prédictions de l'effet de nouvelles conditions de gestion ou d'environnement car ils sont polyvalents et génériques grâce à leur indépendance vis-à-vis des conditions actuelles (Fontes et al., 2010). En raison de la complexité des processus impliqués dans les PBM, ceux-ci ont été initialement utilisés pour modéliser des systèmes relativement simples tels que des plantations monospécifiques et équiennes, mais il existe aujourd'hui plusieurs modèles de peuplements multi-spécifiques et hétérogènes (Mäkelä, 2003;Fontes et al., 2010) qui fonctionnent au moins aussi bien que les modèles empiriques sous conditions actuelles (Fontes et al., 2006;Pinjuv et al., 2006;Miehle et al., 2009).

Les PBM considèrent la plantation soit à l'échelle du peuplement, soit à l'échelle de l'arbre. On parle alors de stand-scale PBM et de tree-scale PBM respectivement. Les stand-scale PBM traitent la forêt comme des couches horizontalement homogènes. Ces modèles génèrent souvent des prédictions moyennées à la parcelle et sont principalement utilisés pour des prévisions quantitatives de la productivité en fonction des sites, des années et du climat (Mäkelä et al., 2000). De plus, ces modèles sont incapables par nature de prendre en compte les distributions spatiales complexes des forêts inéquiennes ou plurispécifiques, ou des systèmes agroforestiers (Porté and Bartelink, 2002).

En revanche, les tree-scale PBM sont des modèles capables de prendre en compte l'hétérogénéité spatiale car ils décrivent et conservent l'emplacement de chaque arbre dans la parcelle considérée (Porté and Bartelink, 2002). Ils sont nécessaires pour tenir compte des diverses compétitions pour la lumière (Porté and Bartelink, 2002;Duursma and Medlyn, 2012b). En principe, ces modèles semblent être les plus pertinents pour la recherche appliquée à la gestion forestière (Seidl et al., 2005), surtout pour des environnements changeants. Mais en raison de leur complexité, ils peuvent avoir des temps de calcul élevés et ils peuvent être difficiles à paramétrer à cause du nombre élevé de paramètres et de leur difficulté d'acquisition. Cependant, Van Oijen et al. (2005) ont utilisé l'inversion bayésienne pour calibrer leur PBM de manière plus simple, mais la procédure est compliquée elle-même, ne supprime pas l'incertitude des paramètres (Fontes et al., 2010) et ajoute une forme d'empirisme au modèle car l'algorithme peut donner des valeurs de paramètres dénuées de sens physique ou physiologique, mais qui donnent de bons résultats *in fine* (pour de mauvaises raisons).

### *Modèles hybrides (HM)*

Un modèle hybride est un modèle issu du couplage de deux modèles. Ce couplage peut se faire de plusieurs manières, et en utilisant des types de modèles différents. Les modèles hybrides sont généralement utilisés pour intégrer des effets à un modèle qu'il ne pourrait pas prendre en compte autrement, comme par exemple des calculs à une échelle plus petite que celle du fonctionnement même du modèle d'origine (Marie et al., 2014), ou des calculs qui prennent en compte de nouveaux compartiments comme le sol par exemple (voir couplage MAESTRA-SPA, Duursma and Medlyn (2012b)). Les PBM intègrent tous pour l'instant des processus issus d'autres modèles, ou des processus statistiques ou mal compris, faisant de chacun d'eux des modèles hybrides dans une certaine mesure.

### *Les modèles de trouées (Gap model)*

Les modèles de trouées sortent un peu du classement EM-PBM-HM (Franc et al., 2000) parce que la plupart ne sont pas spatialement explicites (Porté and Bartelink, 2002). Ces modèles considèrent la forêt comme un regroupement d'arbres en groupes verticalement homogènes et indépendants, d'âge et de stade de succession définis. L'implantation, la croissance et la mortalité de chaque groupe sont simulées en fonction de facteurs biotiques (compétitions) et abiotiques (climat, sol). La mortalité d'un arbre dominant produit un chablis en tombant à terre, aussi appelé trouée (gap), d'où le nom de modèle de trouée (gap model). Ce phénomène est au cœur de la dynamique du modèle, car il va entraîner le recrutement de nouveaux individus qui vont générer des successions (Bugmann, 2001). À l'origine, ils ont été développés pour comprendre la dynamique naturelle à long terme des écosystèmes forestiers naturels plutôt que la croissance et le rendement (Shugart and West, 1981; Bartelink, 2000), mais les développements récents permettent maintenant de simuler des peuplements gérés spatialement hétérogènes (Didion et al., 2009).

### **1.3.3. La modélisation de l'adaptation aux changements climatiques par la gestion**

Plusieurs auteurs ont essayé de décrire ce que doit intégrer au minimum un modèle pour simuler l'effet des changements climatiques et de la gestion sur les plantations pérennes (Weiskittel et al., 2010; Schwalm and Ek, 2001; Landsberg, 2003). On peut considérer que ce modèle devra au moins intégrer des calculs à l'échelle de la journée, une description de l'interception de la lumière qui dépend de la position du soleil, de la structure de la canopée et du type de radiation, un calcul de la photosynthèse basé sur les équations biochimiques de Farquhar et al. (1980), une estimation de la conductance stomatique qui dépend du déficit de pression de vapeur et du statut hydrique du sol, et une prise en compte de la disponibilité en nutriments. C'est pourquoi les modèles qui semblent le mieux adaptés sont les tree-scale PBM (Seidl et al., 2005), même s'il est intéressant de noter que les stand-scale PBM peuvent tout de même prendre en compte certains effets de mélanges d'espèces et certains effets de gestion (Pretzsch et al., 2015).

Les tree-scale PBM ont la particularité d'une part de produire des prédictions qui ne dépendent pas des conditions climatiques actuelles, et d'autre part de mieux prendre en compte les effets de l'hétérogénéité spatiale sur l'interception de la lumière qui est souvent induite par les effets de gestion tels que l'éclaircie, le taillis ou le mélange d'espèces et l'agroforesterie. Ces différences d'interception lumineuse entre individus peuvent ensuite se répercuter sur tous les processus physiologiques des plantes dont la photosynthèse, la transpiration ou encore la température du couvert, et ensuite influencer sur les processus du sol comme l'évaporation ou la température.

De plus, pour mieux intégrer tous les processus importants impliqués dans l'écosystème d'une plantation, un continuum sol-plante-atmosphère, ou SPAC (Philip, 1966), apparaît fondamental. Ce continuum décrit les processus et leurs interactions qui se produisent entre les domaines du sol, de la plante et de l'atmosphère pour représenter l'état de l'écosystème en termes de flux couplés d'eau, de carbone et d'énergie.

En effet, chaque composant est important pour modéliser ces bilans car chacun d'eux peut ensuite influencer en retour les flux des autres par des processus tels que les potentiels hydriques, les phases hydriques et l'énergie disponible (Lobet et al., 2014). Ensuite, la quantité d'énergie entrant dans une composante du système (sol, feuilles, bois...) va dépendre de l'énergie incidente provenant de l'atmosphère sous forme de lumière, ainsi que des propriétés physiques de cette composante telles que son émissivité, sa transmissivité, son absorbance ou sa structure. L'énergie absorbée par un composant est ensuite la source de tout changement potentiel de sa température et de la phase de l'eau à l'intérieur ou à sa surface, déclenchant ainsi l'évaporation de l'eau et/ou la transpiration. Cette énergie absorbée interagit également avec l'air environnant par convection (flux sensible) et vapeur (flux latents par changement de phase), augmentant sa température et son humidité. Les précipitations d'eau vont soit être interceptées par la canopée puis réévaporées, soit atteindre le sol. Une fois le sol atteint, l'eau va soit ruisseler en surface, soit pénétrer le sol et le recharger en eau, ou drainer plus profondément. L'eau a trois moyens de quitter à nouveau le sol : par drainage profond, captée par la plante puis transpirée, ou alors évaporée depuis la couche de surface.

Enfin, les bilans hydriques et énergétiques interagissent à leur tour également avec le cycle du carbone. En effet, les plantes utilisent une partie de l'énergie absorbée pour fabriquer des carbohydrates (sucres) à partir du CO<sub>2</sub> atmosphérique diffusant à travers leurs stomates. Ce faisant, l'eau provenant des stomates s'évapore (*i.e.* transpiration), ce qui conduit à un potentiel hydrique local plus négatif, qui va provoquer un flux d'eau depuis le sol vers les racines puis vers la feuille. Pour éviter la dessiccation, la conductance stomatique peut être ajustée par les plantes selon deux comportements (Tardieu and Simonneau, 1998) : anisohydrique, dans lequel les plantes ne ferment que tardivement leurs stomates, ou isohydrique, lorsque les plantes ferment rapidement leurs stomates par production d'acide abscissique et/ou en réponse au potentiel hydrique foliaire (Tuzet et al., 2003; Tardieu and Davies, 1993; Comstock, 2002). Cependant, la distinction des deux comportements n'est pas très claire, et est sujet à débat car certaines plantes peuvent utiliser l'un ou l'autre suivant la saison, le stade de développement, l'état hydrique du sol, ou le type d'aquaporine exprimé (Ollat et al., 2014).

La fermeture des stomates peut être en fonction de deux facteurs (Tuzet et al., 2003) : le microclimat autour de la feuille, qui dépend lui-même de l'équilibre énergétique du système ; et le potentiel hydrique de la feuille, directement lié au statut hydrique du sol. En contrôlant les flux de carbone dans les plantes, l'énergie et l'eau influent sur leur croissance. Ainsi, le cadre SPAC est complexe car il nécessite une grande quantité de connaissances sur les propriétés physiques et physiologiques du système, mais il est indispensable pour simuler correctement les processus en jeu dans les plantations.

#### **1.4. Problématique et objectifs généraux**

Les effets des changements climatiques vont dépendre de chaque localité, ainsi que de chaque espèce cultivée. Certaines régions vont bénéficier d'un climat plus adapté à la croissance de leurs cultures, quand d'autres verront leurs productions diminuer. Pour prédire le comportement de chaque culture dans chaque localité, il faut des outils capables de prendre en compte tous les processus en jeu, comme l'élévation de la température et

de la concentration en CO<sub>2</sub> atmosphérique, ainsi que les changements de régime de pluies. Une fois les effets connus, les scientifiques, agriculteurs et politiques peuvent alors rechercher, mettre en place et favoriser des solutions d'adaptation des cultures. Ces solutions sont principalement (1) la sélection génétique de souches plus résistantes aux nouvelles conditions ; (2) l'adoption de nouvelles gestions qui permettent d'éviter (*e.g.* changements de calendriers) ou d'atténuer (*e.g.* mélange d'espèces, irrigation, agroforesterie) les effets des changements ; ou encore (3) le changement de culture.

Les plantations pérennes sont peut-être celles qui présentent le plus complexe de ces défis : à cause de leur cycle de vie long, elles ne peuvent pas être adaptées par évitement (*e.g.* semis plus précoce, variétés à cycle court, etc.), et leur adaptation génétique est plus lente que celle des cultures annuelles. De plus, les types de gestion à considérer sont très nombreux, et leurs effets encore peu ou mal évalués car la gestion influe sur l'hétérogénéité de la canopée, qui agit sur des processus à l'échelle de la plante, tels que l'interception de la lumière, la température de canopée, la transpiration, ou encore la photosynthèse.

Par conséquent, nous avons besoin de développer des outils capables de prendre en compte tous les effets des changements climatiques ainsi que de la gestion, à l'échelle où ils agissent pour pouvoir répondre à la problématique générale qui pourrait se résumer à cette question :

**Quels vont être les effets des changements climatiques sur les cultures pérennes, et quel est le potentiel des différentes gestions envisageables pour les adapter ?**

Les objectifs généraux de la thèse peuvent ainsi être déclinés en plusieurs points successifs :

1. Identifier une méthode de modélisation permettant la simulation des effets des changements climatiques sur la production des plantations pérennes, ainsi que l'effet de la gestion comme l'agroforesterie, l'éclaircie, l'émondage, la taille, la densité de plantation, ou l'espèce ;
2. Tester la méthode de modélisation sur des conditions actuelles ou passées pour s'assurer de sa bonne représentation des processus en jeu ;
3. Simuler les plantations pérennes considérées sous changements climatiques pour comprendre et appréhender ses effets ;
4. Simuler différentes gestions de référence ou modifiées pour repérer les gestions les mieux adaptées aux conditions futures, et ainsi évaluer le potentiel de la gestion comme moyen d'adaptation.

## 1.5. Systèmes agricoles choisis pour la thèse

### 1.5.1. *Coffea arabica*

*C. arabica* est originaire des forêts tropicales d'altitude (1600-2800 m) d'Ethiopie, où le climat est relativement stable toute l'année, avec des températures moyennes peu fluctuantes autour de 20°C, et des précipitations entre 1600 et 2000 mm, avec une saison sèche d'approximativement trois à quatre mois (DaMatta and Ramalho, 2006). Ce café est très prisé pour ses qualités stimulantes et gustatives (Cagliani et al., 2013), et sa production représente en 2016 plus de 63% des 9.2 millions de tonnes de café produits dans le monde, dont 42% provenant du Brésil (30%) et de la Colombie (ICO, 2017). Les températures optimales de

croissance de l'arabica sont comprises entre 18 et 21°C, en dessous desquelles la croissance est fortement réduite, et en dessus desquelles la fructification est négativement impactée, d'abord par une maturation trop rapide qui altère la qualité du café, puis par des avortements de bourgeons floraux ou des malformations de fleurs au-dessus de 25.5°C, et enfin un arrêt total de la floraison au-delà d'une température moyenne lors du développement de 30.5°C (DaMatta and Ramalho, 2006; Drinnan and Menzel, 1995; Ramírez, 2009; Rodríguez et al., 2011). Cependant, les températures adéquates changent en fonction du stade phénologique, et des températures plus fortes pourront être tolérées par exemple lors de la germination ou de la croissance de la jeune plante. Les précipitations optimales se trouveraient quant à elles entre 1200 et 1800 mm, avec un période de sécheresse courte entre 2 et 4 mois maximum (DaMatta and Ramalho, 2006). Cette période de sécheresse influence la périodicité de floraison, car la levée de dormance des bourgeons floraux est stimulée par les fortes pluies suivant une sécheresse (Rodríguez et al., 2011). Par exemple, les régions présentant des climats relativement constants avec des températures peu fluctuantes et des pluies distribuées de façon relativement uniforme tout au long de l'année (régions équatoriales, typiquement) auront tendance à présenter des productions étalées dans le temps (*e.g.* Colombie, Zimbabwe), alors que les caféiers plantés dans des régions ayant des saisons plus marquées auront des productions de fruits plus regroupées (typiquement régions subtropicales, *e.g.* Brésil). Cependant, l'effet de la saison sèche est parfois diminué voire absent, et d'autres facteurs pourraient aussi influencer la levée de dormance (Masarirambi et al., 2009).

Etant à l'origine une plante de sous-bois, le café arabica peut être planté sous des arbres d'ombrages en agroforesterie pour imiter son environnement naturel. Cependant, la culture sous ombrage à progressivement été abandonnée au profit de la culture en plein soleil par de nombreux planteurs, notamment au Brésil et en Colombie car la gestion « plein soleil » à tendance à donner de meilleurs rendements (DaMatta et al., 2007). Néanmoins, la culture sous ombrage offre de nombreux avantages pour peu qu'elle soit bien gérée : production moins variable, plus grande biodiversité, bénéfices économiques grâce à la production de bois ou de fruits des arbres d'ombrages, meilleure qualité du café, réduction des extrêmes climatiques, atténuation de la biennialité ou encore une réduction de la transpiration des caféiers (DaMatta et al., 2007; Lin, 2007; Muschler, 2001).

Par conséquent, *C. arabica* est un bon candidat pour étudier les effets des changements climatiques sur les cultures pérennes à fruits car il est très sensible aux températures ainsi qu'aux régimes de précipitations, et est cultivé dans une grande partie du monde. Un de ces avantages est aussi le grand nombre de gestions déjà utilisées de nos jours qui pourraient potentiellement réduire les effets des changements climatiques, notamment grâce à la réduction des températures autour du caféier ainsi que la limitation de sa transpiration grâce à l'ombrage.

### 1.5.2. *Eucalyptus*

Les plantations d'Eucalyptus sont originaires d'Australie, et couvrent aujourd'hui environ 20 millions d'hectares dans le monde, dont 5.6 millions au Brésil (Germon et al., 2017; Booth et al., 2015) qui apportent

5% du PIB national (ABRAF, 2012). Cette essence est cultivée pour produire du bois, et est cultivée au Brésil de manière intensive (rotation courte, plantation clonales, fertilisation, mécanisation, etc.). Les parcelles sont de fait particulièrement homogènes (Lambais et al., 2017). Ces arbres sont parmi les plus productifs au monde grâce à leur forte croissance initiale, et sont ainsi abattus très jeunes entre 5 et 7 ans après plantation (Ryan et al., 2010). Le bois est utilisé principalement pour la production de pâte à papier, de charbon, de panneaux de bois ou de bois de chauffage (Gonçalves et al., 2013). Ces plantations industrielles ont aussi des conséquences importantes sur les écosystèmes, car elles sont souvent plantées à la place de forêts naturelles, ce qui réduit la biodiversité, modifie le cycle de l'eau à cause de leur grande consommation d'eau, et augmente l'érosion et la perte de nutriments si les plantations sont mal gérées (Christina, 2015). Cependant, elles ont un potentiel non négligeable de stockage du carbone dans les sols sous certaines conditions de gestion (Paul et al., 2003).

Les plantations d'Eucalyptus ont donc deux intérêts majeurs pour la modélisation :

- Leur homogénéité structurelle, qui en font un bon système de référence sur un gradient de complexité.
- Leurs flux élevés de carbone et d'eau, utilisés pour tester les limites des modèles.

## 1.6. Sites d'études expérimentaux

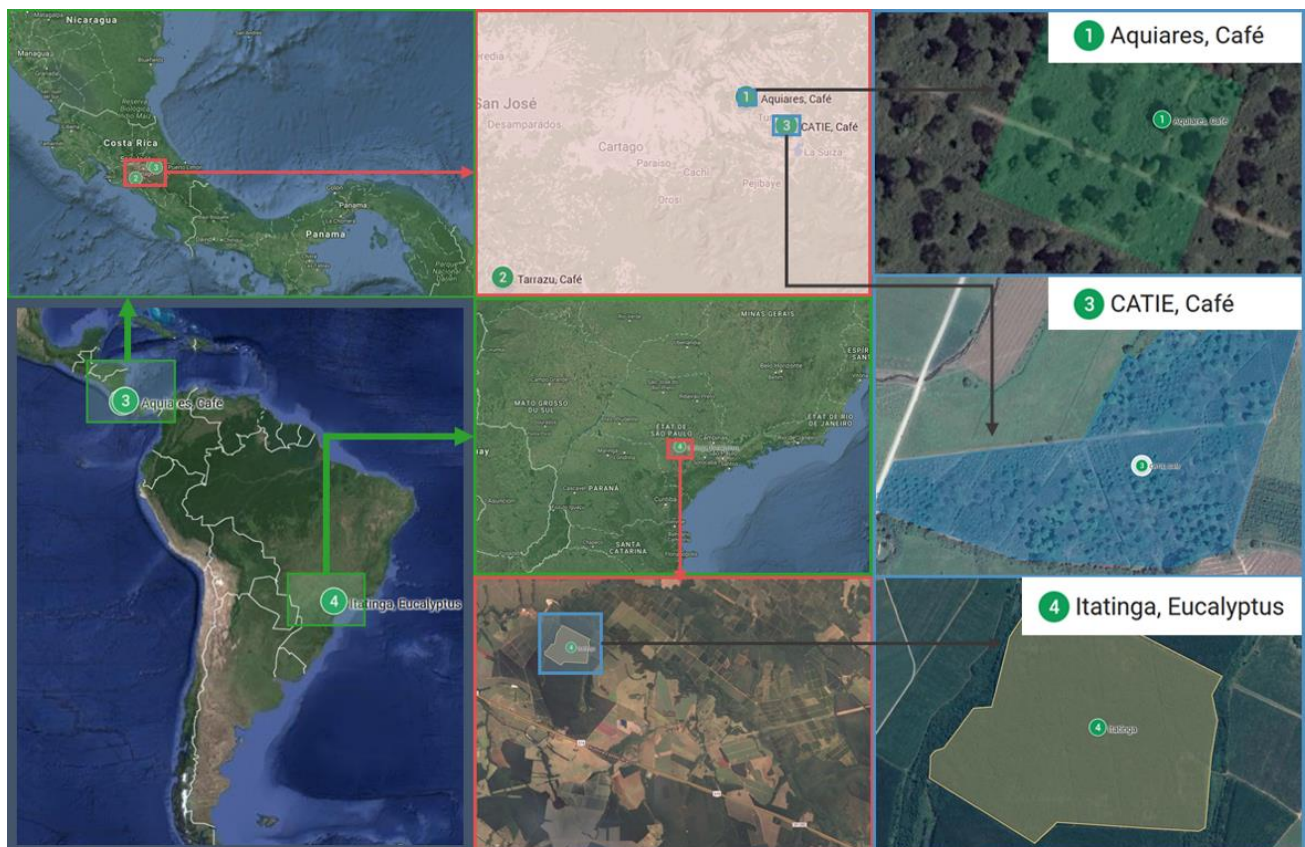


Figure 4. Position géographique des sites d'études expérimentaux utilisés durant la thèse. Les sites d'expérimentations sont visibles en détails à cette adresse : <https://goo.gl/7FRNXg>. 1/ Aquiares, plantation de café en système agroforestier sous Erythrinnes en croissance libre, site CoffeFlux ; 2/ Tarrazu, région de plantation de caféiers en agroforesterie ; 3/ CATIE, essai expérimental de caféiers plantés sous différentes gestions d'ombrage et de fertilisation ; 4/ Itatinga, parcelle d'Eucalyptus du site EucFlux. Source : adapté depuis données cartographiques ©NASA Terrametrics fournies par ©Google.



### 1.6.1. CoffeeFlux, AQUIARES, Costa Rica



**Figure 5. Plantation de café en système agroforestier d'Aquiaries, Costa Rica. Source : Photo F. Beilhe & O. Roupsard.**

Le premier site expérimental est situé dans la ferme d'Aquiaries à 1040 m d'altitude, sur les pentes du volcan Turrialba au Costa Rica (Figure 4, Figure 5). Avec ses 660 ha de caféiers en AFS, la ferme d'Aquiaries est la plus grande plantation certifiée Rainforest Alliance au Costa Rica. Le climat de la région est sous influence caribéenne, avec 3037 mm par an en moyenne entre 2009 et 2015, et une saison sèche relativement courte et peu intense au mois de mars. La température moyenne annuelle se situe autour de 19.5°C. La parcelle d'expérimentation couvre une zone de 1.3 ha, qui est plantée en système agroforestier mélangeant la variété *Caturra* de *Coffea arabica* ainsi que des arbres d'ombrages de l'espèce *Erythrina poeppigiana* plantés en faible densité (7.4 trees ha<sup>-1</sup>) et en croissance libre depuis les années 2000. Cette faible densité d'arbres donne une couverture de canopée d'environ 15% de la parcelle. Les caféiers sont taillés sélectivement selon leur état individuel tous les 5 à 6 ans pour éviter les phénomènes de fatigue des rejets, ce qui en fait une parcelle très hétérogène horizontalement (rejets d'âges différents), ainsi que verticalement (couche de caféier et d'arbres d'ombrages). Cette parcelle est fortement instrumentée depuis 2009 grâce au projet CoffeeFlux (<http://www.umr-ecosols.fr/index.php/en/recherche/projets/53-coffee-flux>). Ont été entre autres mesurés les flux d'eau, de carbone et d'énergie en utilisant la méthode des corrélations turbulentes (Eddy covariance), les températures et le contenu en eau du sol à plusieurs profondeur ou encore les flux de sèves de quelques individus ainsi que leur potentiel foliaire.

Ce site présentant de très nombreuses mesures (flux, productivité primaire nette, rendement, etc.), il a été utilisé pour paramétrer les modèles, puis pour les tester et les valider sur les bilans d'énergie, les bilans de carbone, les bilans hydriques, ainsi que sur production de café à l'échelle de la parcelle. Les données ont été acquises et partagées par l'équipe d'Olivier Roupsard (CIRAD-CATIE).

### 1.6.1. Tarrazu, Costa Rica



Figure 6. Plantations de café dans la région de Tarrazu, Costa Rica. Source : B. Rapidel

Tarrazu est une petite région de production du café de très haute qualité située au Costa Rica qui est située aux alentours de 1500 m d'altitude, à 50 km au sud-ouest d'Aquiaries (Figure 4, Figure 6). Le climat est sous influence pacifique, avec une précipitation moyenne de 1662 mm, et une saison sèche plus marquée de quatre mois approximativement, de Janvier à Avril. Du fait de son altitude plus élevée, la température moyenne annuelle y est aussi plus fraîche, avec 18°C. Cette région présente beaucoup de cultures de café en agroforesterie, avec des caféiers arabica de la variété *Caturra* comme à Aquiaries, plantés principalement sous l'ombrage d'Erythrines, mais aussi sous des bananiers ou d'autres espèces d'arbres. D'autres parcelles sont aussi plantées en plein soleil.

Ce site est principalement utilisé comme second site de référence pour les prédictions de production de café à long terme, car il dispose d'un climat relativement différent de celui d'Aquiaries. Les données ont été acquises et partagées par l'équipe de Bruno Rapidel (CIRAD-CATIE).



### 1.6.2. CATIE, Costa Rica



Figure 7. Plantations de café en AFS de l'essai expérimental du CATIE, Costa Rica. Source : E. de Melo.

Le site du CATIE est une parcelle d'expérimentation de 9 ha plantée en 2000 à 10 km au sud-est de la plantation d'Aquiaries, et qui vise à tester l'effet de l'ombrage et de la fertilisation sur les caféiers (Figure 4, Figure 7). Le climat est tropical humide sous influence caribéenne comme à Aquiaries. Mais son altitude étant plus basse (685 m), sa température moyenne est plus élevée (23°C), et à la limite des conditions de culture du café arabica. Il pleut environ 2700 mm par an, et la saison sèche est très réduite, de un mois environ.

Les niveaux d'ombrages sont modulés de la façon suivante : pas d'ombrage (en plein soleil), sous une espèce d'arbre d'ombrage, ou sous un mélange de deux espèces d'arbres, plantés selon une grille de 4\*6 m initialement, puis éclaircis par la suite. Les 645 arbres d'ombrages sont répartis en trois espèces différentes : *Chloroleucon eurycyclum*, un arbre géré en croissance libre avec une grande capacité de couverture et qui a la capacité de fixer l'azote atmosphérique ; *Terminalia amazonia*, une espèce aussi en croissance libre, avec une canopée haute et compacte ; et *Erythrina poeppigiana*, une espèce fixatrice d'azote qui est ici émondée à 3-4 m deux fois par an pour moduler le niveau de lumière arrivant à la couche de caféier selon son stade phénologique. Le site dispose donc d'une végétation à la structure très hétérogène spatialement, autant horizontalement que verticalement.

Deux variables intéressantes ont été mesurées sur ce site : la transmittance de la lumière au-dessus des caféiers (2 m du sol) sous la canopée des différents arbres d'ombrages ou en plein soleil, et la température de canopée de plants de caféiers sous les différentes gestions d'ombrage. Ces mesures ont permis de tester et valider le modèle utilisé pour la simulation de l'interception de la lumière et de la température de canopée. Les données ont été acquises et partagées par l'équipe de Elias de Melo (CATIE). La méthodologie d'acquisition des données est détaillée dans l'article de Soma et al. (in prep.), qui est joint au manuscrit en Annexe 1.

### 1.6.3. EucFlux, Itatinga, SP-Brésil



**Figure 8.** Plantation d'Eucalyptus du site EucFlux, Itatinga, SP Brésil. Source : A. Germon.

La station expérimentale du département des sciences forestières de l'université de São Paulo est située près de la ville d'Itatinga, dans l'état de São Paulo au Brésil. Une parcelle expérimentale d'*Eucalyptus urophylla x grandis* (Figure 8) fut plantée en 2009 à environ 13 kilomètres de la station dans le cadre du projet EucFlux (<http://www.ipef.br/eucflux/en/>). Sur ce site, les précipitations annuelles totalisent en moyenne 1360 mm, et la température moyenne annuelle est d'environ 20 °C, avec une variabilité de 5°C entre les deux saisons relativement marquées (15°C de juin à septembre, 25°C d'octobre à mars). D'une densité de 1666 arbres ha<sup>-1</sup> (plantation en lignes de 2\*3 m), les Eucalyptus forment une canopée très homogène. Le site est fortement instrumenté, et dispose de mesures météorologiques complètes, mais aussi des mesures de flux de carbone, d'eau et d'énergie grâce à la méthode des corrélations turbulentes (Eddy covariance), un suivi du contenu en eau du sol jusqu'à 10 mètres de profondeur, des mesures de biomasses destructives précises et régulières, et bien d'autres.

Ce site permet de tester le modèle sur une plantation homogène, ainsi que de tester la généralité du modèle entre des écosystèmes très contrastés « monoculture eucalyptus » et « agroforestiers café ». Les données ont été acquises et partagées par l'équipe de Jean-Paul Laclau, Yann Nouvellon, Jean-Pierre Bouillet et Gueric le Maire (CIRAD).

## 1.7. Approche de modélisation numérique retenue

L'objectif de la modélisation est de simuler l'impact des changements climatiques sur les cultures de café des sites de Tarrazu et d'Aquiara, ainsi que d'expérimenter le potentiel d'adaptation de différents types de gestion. A cet effet, le modèle choisi doit (1) être capable de représenter correctement les processus potentiellement impactés par les changements climatiques (CO<sub>2</sub>, température, bilan d'eau, de carbone et d'énergie) ; (2) être capable de représenter correctement les processus potentiellement impactés par la gestion comme

l'interception lumineuse, l'efficacité d'utilisation de la lumière, le microclimat ou l'évapotranspiration et (3) être assez rapide pour pouvoir simuler de longues périodes (>100 ans) et de nombreux scénarios de gestions et de climats sur des sites différents.

### 1.7.1. Modélisation tridimensionnelle : MAESPA

MAESPA (Duursma and Medlyn, 2012b) est un modèle basé sur des processus physiques et physiologiques fins qui simule les flux d'énergie, de carbone et d'eau d'écosystèmes forestiers. Le pas de temps du modèle est infra-horaire. L'unité de simulation spatiale est celle de la parcelle pour les processus du sol, et celle du voxel pour les plantes, qui est une discrétisation de l'espace en volumes supposés homogènes et représentatifs des différentes parties de la canopée d'un individu. Chaque arbre dans la plantation est décrit individuellement, avec son propre jeu de paramètres de structure (*e.g.* coordonnées spatiales, hauteur, largeur, forme de couronne, aire foliaire), de physiologie (*e.g.* classe d'âge, paramètres de conductance et de photosynthèse...) et de caractéristiques optiques (réflectance et transmittance des feuilles).

Ce modèle est particulièrement bien adapté à la modélisation de systèmes spatialement hétérogènes comme les AFS car il décrit la plantation en trois dimensions, et peut donc estimer les variables impactées à l'échelle de la plante comme l'interception lumineuse ainsi que l'hétérogénéité de la distribution de la température de canopée, qui vont toutes deux influencer les bilans de carbone, d'eau et d'énergie. Il peut donc aussi être utilisé pour l'étude des effets de la gestion sur la plantation. De plus, comme il décrit les processus écophysologiques de façon mécaniste, il est également bien adapté à la simulation des effets des changements climatiques.

Enfin, ce modèle a déjà été paramétré et utilisé pour la simulation de plantations d'Eucalyptus (Christina, 2015;Christina et al., 2017;Christina et al., 2016;Christina et al., 2015;le Maire et al., 2013;Medlyn et al., 2007;Duursma and Medlyn, 2012), ainsi que sur une plantation de caféier en agroforesterie (Charbonnier et al., 2017;Charbonnier, 2013;Charbonnier et al., 2013). Cependant, MAESPA ne dispose pas de modules d'allocation du carbone et de croissance, et requiert des calculs intensifs liées à sa représentation tridimensionnelle. Il n'est donc pas très adapté pour une application à des simulations sur des durées de plusieurs années, voire décennies. Le modèle est décrit plus en détail dans le Chapitre 2.

### 1.7.2. Modèle dynamique de culture (dynamic crop model : DCM)

A notre connaissance durant la période de la thèse, deux modèles dynamiques basés sur des processus étaient disponibles dans la littérature pour simuler les caféiers :

- Un modèle dynamique de caféier isolé de plein soleil (Rodríguez et al., 2011) : ce modèle est basé sur des processus, il fonctionne aux échelles du nœud fructifère, du rameau et de la plante entière. Il est très détaillé pour le cycle de reproduction et a été vérifié sur des jeux de données provenant de sites équatoriaux et subtropicaux (nécessitant une recalibration des paramètres). Toutefois, il n'a été testé



qu'entre le jour de plantation et cinq ans après la plantation, et ne permet pas une utilisation sur une parcelle agroforestière car c'est un modèle à l'échelle de la plante isolée, et non de la parcelle.

- Un modèle dynamique de parcelle de café agroforestier (Van Oijen et al., 2010b) : il s'agit d'un modèle basé sur des processus, fonctionnant à l'échelle de la parcelle entière, permettant de calculer les flux, la croissance et de nombreux services écosystémiques entre des zones sous arbre d'ombrage et des zone hors arbre d'ombrage. Bien que très polyvalent, ce modèle présente quelques inconvénients : un calcul approximatif de l'interception lumineuse lié au fait que ses calculs soient à l'échelle de la sous-parcelle (ombragée ou plein soleil), un calcul descriptif de la température de canopée au lieu d'un calcul mécaniste, une efficacité de l'utilisation de la lumière constante, pas de calcul de bilan d'énergie, et enfin, aucune publication n'est disponible sur la vérification du modèle sur des données de croissance ou de production.

Nous avons donc opté pour le développement d'un modèle dynamique combinant les avantages de ces deux modèles (Tableau 1) :

- Un calcul des variables influencées par la structure de la canopée et le climat à l'échelle de l'individu grâce à l'utilisation de métamodèles de MAESPA (voir paragraphe 1.7.3), intégrées dans l'espace agroforestier via des métamodèles ;
- Une échelle de travail parcelle agroforestière, au pas de temps journalier, en séparant la couche caféier de la couche d'arbre. Chaque couche est en réalité une plante moyenne, résultant de l'intégration de l'hétérogénéité à l'échelle parcelle ;
- Un calcul de la phénologie capable de prendre en compte le développement reproductif complexe du caféier grâce à l'intégration de cohortes de bourgeons et de fleurs basé sur le modèle de Rodríguez et al. (2011), intégré à l'échelle de la plante pour éviter les calculs fastidieux à l'échelle du nœud ou du rameau et permettre des vérifications à l'échelle de la plante ou de la parcelle ;
- Un calcul simple mais efficace des bilans hydriques du sol par l'intégration du modèle BILJOU (Granier et al., 2012).
- Un calcul de services écosystémiques, moins polyvalent mais plus précis que dans Van Oijen et al. (2010b).

Le modèle est décrit en détail dans le Chapitre 3.

**Tableau 1. Caractéristiques comparées de trois modèles dynamiques basés sur des processus appliqués au caféier.**

<b>Caractéristique</b>	<b>Rodríguez et al. (2011)</b>	<b>Van Oijen et al. (2010b)</b>	<b>Notre modèle</b>
Basé sur des processus	Oui	Oui	Oui
Echelle de travail et des données pour vérification	Rameau à plante entière	Sous-parcelle <sup>(1)</sup>	De la plante à la parcelle
Compatible agroforesterie	Non	Oui	Oui
Validé sur des données de terrain	Oui	Non (O. Ovalle y travaille)	Oui
Hétérogénéité et phénomènes non-linéaires intra-parcelle <sup>(2)</sup>	Non	Non	Oui, via métamodèles de MAESPA
Compartiment de réserves	Non	Non	Oui
Biennialité dynamique	Oui	Non	Oui
Simulation de rotations entières	Non	Oui	Oui
Simulation sous changements climatiques	Non	Oui	Oui
Doit être recalibré sur chaque site d'étude	Oui	Pas d'information publiée	Oui
Phénologie de la reproduction détaillée	Oui	Non	Oui, dérivé de Rodríguez et al. (2011)
Cohortes de fruits explicites	Oui	Non	Oui
Floraison basée sur un process model	Oui	Non (forcée et synchrone)	Oui
Maladies	Oui, Coffee Berry Borer	Non	Oui, American Leaf Spot (Mycena)
Température de canopée pour le développement de la plante	Non (Tair)	Non (Tair)	Oui
Augmentation de la LUE à l'ombre (Charbonnier et al., 2017)	Non	Non	Oui

(1) : Dichotomie plein soleil / sous arbre d'ombrage

(2) : *e.g.* lumière, température, humidité, LUE, k, température de canopée

### 1.7.3. Métamodèles

Pour développer un modèle dynamique de culture fonctionnant à l'échelle de la parcelle mais qui puisse tout de même calculer les variables dépendantes de la structure de la canopée et du climat à l'échelle où elles sont affectées, c'est-à-dire à l'échelle temporelle infra-journalière et à l'échelle spatiale de l'individu, nous avons choisi d'utiliser des métamodèles de MAESPA. Les métamodèles sont des modèles statistiques simples et instantanés qui sont entraînés à reproduire les sorties d'un modèle depuis ses variables d'entrées, à la même échelle de travail, ou à une échelle moins fine (Faivre et al., 2013). Ils sont en quelque sorte un résumé du modèle complexe car ils ne prennent pas en compte explicitement les processus développés dans le modèle d'origine. Ces métamodèles peuvent ensuite être utilisés comme tels, ou intégrés très facilement dans d'autres modèles. En effet, pour peu que le modèle complexe soit déjà paramétré, ils sont ensuite rapides à implémenter, réduisent la complexité du modèle d'origine et sont bien plus rapide car ils peuvent résumer des processus très complexes en une seule équation. De plus, les métamodèles donnent généralement des résultats ayant des erreurs très faibles comparativement au modèle d'origine (Marie et al., 2014; Christina et al., 2016). Cette méthodologie provient du milieu de l'ingénierie, mais est de plus en plus utilisée en environnement pour la modélisation des milieux forestiers, comme par exemple pour les calculs de l'interception lumineuse (Marie et al., 2014), de la prédiction de biomasse (de-Miguel et al., 2014), de changements d'utilisation des terres (Gilliams et al., 2005), ou d'analyses de sensibilité de modèles complexes (Christina et al., 2016).

## 1.8. Objectifs spécifiques de la thèse et démarche suivie

Plusieurs hypothèses de travail ont été formulées au départ de la thèse. La première étant que comparativement aux modèles PBM 1D ou 2D, les modèles PBM 3D sont capables de mieux représenter les effets des changements climatiques et de gestion, particulièrement pour les plantations spatialement hétérogènes comme les AFS. Le modèle MAESPA a été choisi pour ce travail. Cependant, ces modèles sont trop lents pour être appliqués sur de longues séries temporelles, mais un couplage de modèles d'échelles différentes devrait répondre à cette problématique, tout en gardant la précision du modèle complexe. Par conséquent, un modèle dynamique de culture a été développé puis couplé à MAESPA grâce à des métamodèles. La seconde hypothèse principale est que les effets des changements climatiques vont négativement impacter la production de café à long terme principalement à cause d'avortements floraux, mais que l'augmentation de l'ombrage peut atténuer les effets climatiques tout en maintenant des niveaux de photosynthèse suffisants grâce à l'augmentation de la [CO<sub>2</sub>] atmosphérique. La simulation de la température, et en particulier des changements de température des caféiers en fonction des caractéristiques de l'ombrage, est donc d'une importance cruciale dans ce type de modèle.

La démarche suivie peut donc se résumer en quatre points :

- 1- Modification du modèle MAESPA pour un meilleur calcul des températures des feuilles et des températures de l'air dans le couvert, puis paramétrage de MAESPA et évaluation des bilans d'eau et d'énergie du modèle sur deux sites contrastés par leur climat et leur gestion pour valider le modèle

- (Chapitre 2 + étude complémentaire avec Soma et al. (in prep.) et participation à l'étude de Christina et al. (submitted) ;
- 2- Développement et paramétrage du modèle dynamique de culture et couplage avec les métamodèles issus de MAESPA (Chapitre 3) ;
  - 3- Evaluation du modèle de dynamique de culture sur les données du site instrumenté d'Aquières (Chapitre 3) ;
  - 4- Utilisation du modèle dynamique de culture sous différents scénarios de climats futurs et de gestions de l'ombrage (Chapitre 4).

Chacun des 3 chapitres correspond à un article en premier auteur. Le premier a été soumis à *Agricultural and Forest Meteorology* en Aout 2017 (actuellement under review). Les deux autres seront soumis en 2018. Un résumé de l'article en français est donné en début de chaque chapitre. J'ai également participé à deux autres articles soumis ou en préparation, qui sont donnés en annexe de cette thèse (Soma et al., in prep.; Christina et al., submitted). J'ai aussi présenté mes résultats lors de plusieurs conférences (JEF 2017, EURAF 2016, 32<sup>nd</sup> Conference on Agricultural and Forest Meteorology). Le dernier chapitre de la thèse est une synthèse dans laquelle les résultats obtenus sont discutés et mis en perspectives les uns avec les autres, puis où sont présentés de possibles perspectives à ces travaux.







# Chapitre 2. Measuring and modelling energy partitioning in canopies of varying complexity using MAESPA model

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## 2.1. Introduction au chapitre 2

Ce chapitre décrit la première partie du travail de modélisation de la thèse, qui consistait en la modification du modèle MAESPA pour intégrer un calcul de la température et de la pression de vapeur de l'air à l'intérieur de la canopée afin de mieux décrire les échanges d'eau et d'énergie dans cet espace. Le modèle a ensuite été paramétré et utilisé sur trois sites distincts pour procéder à la validation de la modélisation de plusieurs processus agissant à différentes échelles, et sur des systèmes de structure simple et complexe. Ainsi, le modèle a été testé sur une plantation d'Eucalyptus au Brésil pour ces flux d'énergie et d'eau à l'échelle de la parcelle ( $R_n$ ,  $H$ ,  $LE$ ,  $AET$ ). Ce système est relativement simple de structure car la canopée de la plantation est très homogène puisque les arbres sont issus d'un même clone, ont le même âge, et sont plantés selon une grille de 2x3 mètres. Ensuite, le deuxième site, une plantation de caféier en agroforesterie au Costa Rica, a permis de valider MAESPA sur les mêmes flux mais sur une plantation complexe, du fait de la grande hétérogénéité de sa canopée. Enfin, le modèle a été testé pour ses calculs d'interception lumineuse et de température de feuilles à l'échelle de l'individu sur un système encore plus complexe : un site d'expérimentation de l'effet de l'ombrage sur les caféiers, qui comprend des parcelles de caféier cultivés en plein soleil, des parcelles sous arbres d'ombrage laissés en croissance libre ou émondés à 4 m de hauteur, et des parcelles de mélange d'espèces d'arbres et de gestion.

Ce travail nous a donc servi à paramétrer, améliorer et tester MAESPA pour des processus et des conditions variées, et ainsi valider son bon fonctionnement pour son application sur de nouveaux climats et de nouvelles gestions.

Le code du modèle est disponible en accès libre sur le site d'hébergement Bitbucket, dans la branche "Montpellier\_2" du dépôt officiel du modèle MAESPA :

[https://bitbucket.org/remkoduursma/maespa/src/d47aef539b62aaf59df872dc45cbbe120718f7b4?at=montpellier\\_2](https://bitbucket.org/remkoduursma/maespa/src/d47aef539b62aaf59df872dc45cbbe120718f7b4?at=montpellier_2) ou : <https://goo.gl/ti2XEM>

Par ailleurs, un site web dédié à la communication interactive des résultats de la validation du modèle est disponible à cette adresse : [https://vezy.github.io/MAESPA\\_Validation/](https://vezy.github.io/MAESPA_Validation/)

Le site officiel du modèle MAESPA qui est maintenu par Remko Duursma et Belinda Medlyn est disponible à cette adresse : <https://maespa.github.io/>

## 2.2. Résumé en français

Le partitionnement de l'évapotranspiration et de l'énergie entre les différents compartiments de l'écosystème peut être difficile à estimer car il résulte de l'interaction de nombreux processus, en particulier dans les écosystèmes multi-espèces et multi-strates. Nous avons utilisé le modèle mécaniste 3D MAESPA, qui modélise le couplage du transfert radiatif, de la photosynthèse, et des bilans d'énergie et d'eau, pour simuler la répartition de l'énergie et de l'évapotranspiration dans des plantations homogènes, ainsi que dans des systèmes agroforestiers hétérogènes multi-espèces de diverses complexités et gestions. Le modèle MAESPA a été modifié pour ajouter (1) un calcul de l'évaporation de l'eau à la surface des feuilles à l'échelle du voxel ; (2) un

calcul d'une moyenne de température et de pression de vapeur de l'air à l'intérieur de la canopée ; et (3) l'utilisation des points (1) et (2) dans les calculs itératifs de la température du sol et des feuilles pour fermer les bilans d'énergie au niveau de l'écosystème. Nous avons ensuite testé le modèle MAESPA sur un peuplement monospécifique d'Eucalyptus au Brésil, ainsi que dans deux systèmes agroforestiers complexes et hétérogènes de café au Costa Rica. MAESPA simule de manière satisfaisante la dynamique quotidienne et saisonnière du rayonnement net (RMSE = 31.2 et 28.4 W m<sup>-2</sup>, R<sup>2</sup> = 0.98 et 0.98 pour les sites d'Eucalyptus et de café respectivement) et sa répartition entre les flux de chaleur latente (RMSE = 70.2 et 37.2 W m<sup>-2</sup> R<sup>2</sup> = 0.88 et 0.84) et sensible (RMSE = 61.3 et 45.8 W m<sup>-2</sup>, R<sup>2</sup> = 0.61 et 0.82) sur une simulation d'un an avec un pas de temps d'une demi-heure. Après validation, nous utilisons la version modifiée de MAESPA pour estimer la répartition de l'évapotranspiration et de l'énergie entre les plantes et le sol de chaque agroécosystème. Dans la plantation d'Eucalyptus, 95% de l'énergie sortante était émise sous forme de flux de chaleur latente, tandis que la répartition entre les flux de chaleur sensible et latente était à peu près égale dans la plantation de café. Nous concluons que le modèle MAESPA présente un certain équilibre entre finesse de description des processus et rapidité de calcul, et qu'il est donc applicable aux écosystèmes forestiers simples ou complexes à différentes échelles.

1 **2.3. Article scientifique**

2 **Research Paper**

3

4 **Measuring and modelling energy partitioning in canopies of**  
5 **varying complexity using MAESPA model**

6 Rémi Vezy<sup>a,b,c\*</sup>, Mathias Christina<sup>a,b,d</sup>, Olivier Roupsard<sup>a,b,e</sup>, Yann Nouvellon<sup>a,b,f</sup>, Remko Duursma<sup>g</sup>, Belinda  
7 Medlyn<sup>g</sup>, Maxime Soma<sup>a,b,h</sup>, Fabien Charbonnier<sup>a,b,i</sup>, Céline Blitz-Frayret<sup>a,b</sup>, José-Luiz Stape<sup>j</sup>, Jean-Paul  
8 Laclau<sup>a,b,f</sup>, Elias de Melo Virginio Filho<sup>e</sup>, Jean-Marc Bonnefond<sup>c</sup>, Bruno Rapidel<sup>e,k</sup>, Frédéric Do<sup>b,l</sup>, Alain  
9 Rocheteau<sup>b,l</sup>, Delphine Picart<sup>c</sup>, Carlos Borgonovo<sup>m</sup>, Denis Loustau<sup>c</sup>, Gueric le Maire<sup>a,b,n</sup>

10 <sup>a</sup>CIRAD, UMR Eco&Sols, F-34398 Montpellier, France.

11 <sup>b</sup>Eco&Sols, Univ Montpellier, CIRAD, INRA, IRD, Montpellier SupAgro, Montpellier, France

12 <sup>c</sup>INRA, UMR 1391 ISPA, F-33140 Villenave d'Ornon, France

13 <sup>d</sup>CIRAD, UR 115, AIDA, 34398 Montpellier, France

14 <sup>e</sup>CATIE, Centro Agronómico Tropical de Investigación y Enseñanza, Turrialba 30501, Costa Rica

15 <sup>f</sup>Universidade de São Paulo, SP, Brazil

16 <sup>g</sup>Hawkesbury Institute for the Environment, Western Sydney University, Locked Bag 1797, Penrith, NSW 2751,  
17 Australia

18 <sup>h</sup>INRA, UR 629, Ecologie des Forêts Méditerranéennes, Domaine Saint-Paul, 84917, Avignon, France

19 <sup>i</sup>El Colegio de la Frontera Sur, CONACyT research fellow, San Cristóbal de las Casas, 29290 Chiapas, México

20 <sup>j</sup>Suzano Pulp and Paper, Suzano 08613-900, Brazil

21 <sup>k</sup>CIRAD, UMR System, 34060 Montpellier, France

22 <sup>l</sup>IRD, UMR Eco&Sols, F-34398 Montpellier, France

23 <sup>m</sup>Cafetalera Aquiares S.A., PO Box 362-7150 Turrialba, Costa Rica

24 <sup>n</sup>UNICAMP, NIPE, Campinas, Brazil

25 \*Corresponding author. Email address: remi.vezy@cirad.fr (R. Vezy).

26

27

28 **Abstract**

29 Evapotranspiration and energy partitioning are complex to estimate because they result from the interaction of  
30 many different processes, especially in multi-species and multi-strata ecosystems. We used MAESPA model,  
31 a mechanistic, 3D model of coupled radiative transfer, photosynthesis, and balances of energy and water, to  
32 simulate the partitioning of energy and evapotranspiration in homogeneous tree plantations, as well as in  
33 heterogeneous multi-species, multi-strata agroforests with diverse spatial scales and management schemes.  
34 The MAESPA model was modified to add (1) calculation of foliage surface water evaporation at the voxel  
35 scale; (2) computation of an average within-canopy air temperature and vapour pressure; and (3) use of (1)  
36 and (2) in iterative calculations of soil and leaf temperatures to close ecosystem-level energy balances. We  
37 tested MAESPA model simulations on a simple monospecific *Eucalyptus* stand in Brazil, and also in two  
38 complex, heterogeneous *Coffea* agroforests in Costa Rica. MAESPA satisfactorily simulated the daily and  
39 seasonal dynamics of net radiation (RMSE= 31.2 and 28.4 W m<sup>-2</sup>; R<sup>2</sup>= 0.98 and 0.98 for *Eucalyptus* and  
40 *Coffea* sites respectively) and its partitioning between latent- (RMSE= 70.2 and 37.2 W m<sup>-2</sup>; R<sup>2</sup>= 0.88 and  
41 0.84) and sensible-energy (RMSE= 61.3 and 45.8 W m<sup>-2</sup>; R<sup>2</sup>= 0.61 and 0.82) over a one-year simulation at  
42 half-hourly time-step. After validation, we use the modified MAESPA to calculate partitioning of  
43 evapotranspiration and energy between plants and soil in the above-mentioned agro-ecosystems. In the  
44 *Eucalyptus* plantation, 95% of the outgoing energy was emitted as latent-heat, while the *Coffea* agroforestry  
45 system's partitioning between sensible and latent-heat fluxes was roughly equal. We conclude that MAESPA  
46 process-based model has an appropriate balance of detail, accuracy, and computational speed to be applicable  
47 to simple or complex forest ecosystems and at different scales for energy and evapotranspiration partitioning.

48

49 Keywords: partitioning; evapotranspiration; energy; MAESPA; agroforestry system; process-based model.

50

## 51 **1. Introduction**

52 Climate change's multiple, interacting drivers and effects include changes to patterns of temperature and  
53 rainfall, in addition to an increase in atmospheric CO<sub>2</sub> concentration. There is an increasing need for  
54 information to better predict future climate change impacts on perennial crops and forests and to design new  
55 agricultural and silvicultural practices to cope with these changes (Brisson et al., 2010; Ray et al., 2012). All of  
56 those changes lead to complex combinations of effects on the water and carbon balances of ecosystems, and  
57 can thus, potentially, affect agro-ecosystem production (Way et al., 2015). Therefore, agronomists and  
58 foresters must be prepared to design new agricultural and silvicultural practices to cope with impacts of  
59 climate change upon perennial crops and forests. Of critical importance to that design process will be an  
60 understanding of climate change's effects upon ecosystems' water balances. Armed with that understanding,  
61 managers could adapt their practices to future changes in temperature and rainfall patterns (Fischer et al.,  
62 2007) in order to limit the environmental impacts of agricultural systems on aquifers (Christina et al., 2017),  
63 or to reduce erosion while maintaining or increasing crop production (Lal, 1998). However, in-situ  
64 measurements of the main fluxes are difficult and costly, and are possible only at a few, highly-instrumented  
65 sites. While long-term monitoring of evapotranspiration can be done through eddy-covariance techniques, the  
66 other main components (*e.g.*, soil evaporation, plant transpiration, and wet foliage evaporation) remain  
67 difficult to measure directly over long periods (see Kool et al. (2014) for an extended review). Numeric  
68 process-based simulation models (PBMs) are useful to address such challenges.

69 PBMs apply our understanding of fundamental physical and ecophysiological processes (*e.g.*, photosynthesis  
70 and respiration) to simulate the system mechanistically (Bohn et al., 2014). They can be used to estimate  
71 fluxes and stocks of energy, water, and carbon in the ecosystem, as a function of climate, soil, and plant  
72 characteristics. The processes that may need to be modelled in order to understand a phenomenon of interest  
73 depend upon the studied spatial scale, which may range from an individual tree up to the scale of a plot, the  
74 surrounding watershed, the landscape, or the encompassing region (Bayala et al., 2015). Therefore, it is  
75 important that the process-based-modelling community develop and have access to a range of models, with  
76 different degrees of complexity, regarding the question under consideration (Pretzsch et al., 2015). Quite  
77 often, practical considerations impose trade-offs between scale and complexity. As an example of how the  
78 required trade-offs might be made successfully, consider the simulation of heterogeneous stands of trees.  
79 Radiation interception and microclimate (*i.e.* the microclimate below, above or within the canopy and soil) are  
80 two key processes that must be carefully accounted for in those simulations (Charbonnier et al.,  
81 2013; Luedeling et al., 2016; Singh et al., 2012) because they become more heterogeneous as the canopy  
82 structure becomes more complex. Multi-layer models struggle to simulate the light interception of such  
83 ecosystems (Luedeling et al., 2016), which propagate into simulations errors of transpiration and  
84 photosynthesis. For these reasons, tree-level models are more appropriate, and more accurate, than multi-layer  
85 models for simulating horizontally heterogeneous (*e.g.* agroforestry) stands (Seidl et al., 2005). However, few  
86 tree-scale models combine a precise radiation transfer model at the tree scale with fast computation of stand-



87 scale outputs thus allowing easy spatial and temporal extrapolation of a wide range of tree systems (Way et  
88 al., 2015;Flerchinger et al., 2015;Simioni et al., 2000;Simioni et al., 2016). One way to achieve an acceptable  
89 trade-off between accuracy and speed of calculation, in the case of horizontally heterogeneous stands, is by  
90 parameterizing tree-scale models through simplified tree architecture using pseudo-turbid representations of  
91 vegetation canopies instead of leaves and branches (Widlowski et al., 2014). As modelled according to that  
92 architecture, a tree is a set of voxels, each of which represents a certain volume element of the tree foliage.  
93 One model that uses voxels to make the required trade-off between computation time and precision is  
94 MAESPA (Duursma and Medlyn, 2012b), which is a recent coupling of the tree-scale light interception and  
95 ecophysiology model MAESTRA (Medlyn, 2004;Wang and Jarvis, 1990) and the soil and ecosystem water  
96 and energy balance SPA (Williams et al., 2001). MAESPA occupies a very interesting niche in the PBM  
97 complexity continuum, between the complex, detailed 3-D models (Bailey et al., 2016;Disney et al., 2006)  
98 and the less-detailed multi-layer models (Hanson et al., 2004). Thus, MAESPA is a relevant candidate for  
99 addressing effects of climate change upon horizontally heterogeneous forest systems. Indeed, the MAESTRA  
100 component of MAESPA computes 3D-explicit directional light interception at the voxel scale, while also  
101 using a faster “equivalent horizontal canopy” modelling approach similar that used in multilayer models to  
102 compute both the scattered radiation that reaches each voxel (Norman, 1979) and the thermal-radiation  
103 transfer among voxels. MAESTRA then computes main ecophysiological processes at the voxel scale, such as  
104 the net radiation, the absorbed photosynthetically active radiation (PAR), and subsequently photosynthesis and  
105 transpiration. The coupling with SPA model allows a precise computation of soil water balance (using the  
106 Richards equation) and plant hydraulics, so that stomatal conductance can respond to leaf water potential. The  
107 energy balance at the voxel scale is calculated iteratively to equilibrate leaf temperatures. Recent changes to  
108 MAESPA’s soil water balance are described in Christina et al. (2017).

109 MAESPA has been used extensively (<https://maespa.github.io/bibliography.html>) and improved over the past  
110 30+ years, mainly for radiation and CO<sub>2</sub> fluxes. While the model successfully simulated plant transpiration in  
111 a native *Eucalyptus* forest (Medlyn et al., 2007) and a planted *Eucalyptus* stand (Christina et al.,  
112 2017;Christina et al., 2016), it has also been found to under-estimate high evapotranspiration rates on *Coffea*  
113 agroforestry systems (Charbonnier, 2013), and on *Pinus* and *Eucalyptus* stands (Moreaux, 2012). Preliminary  
114 investigations suggested that the underestimation of evapotranspiration in these systems could occur due to  
115 unreliable estimation of canopy temperature. Leaf temperatures were found to be underestimated by several  
116 degrees Celsius under high radiation and evapotranspiration conditions (Charbonnier, 2013). Modeled leaf  
117 temperature remained unrealistically close to air temperature within the canopy, itself remaining equal to the  
118 air temperature given as input to the model, generally taken from a meteorological station located outside the  
119 canopy. Similarly, the vapour pressure (VP) of the canopy airspace is assumed to equal that outside the  
120 canopy.

121 In this paper, we modify the original MAESPA version (Duursma and Medlyn, 2012) to include calculation of  
122 spatially constant values of within-canopy air temperature ( $T_{air_{canopy}}$ ) and within-canopy VP ( $VP_{air_{canopy}}$ ).

123 Both of those variables are calculated from ecosystem-level energy balances. Since  $T_{air_{canopy}}$  and  $V_{Pair_{canopy}}$   
124 result from and in turn affect complex interactions among the canopy, the soil, and the atmosphere above the  
125 canopy, inclusion of  $T_{air_{canopy}}$  and  $V_{Pair_{canopy}}$  is a critical improvement to the MAESPA model. We  
126 hypothesized that that improvement would better simulate a stand's energy balance, including latent- and  
127 sensible-fluxes from trees and soil; air canopy VP and temperature; leaf and soil temperatures; soil water  
128 content; and thus, the stand's water balance.

129 Some models include detailed calculations of canopy turbulence, a key phenomenon that influences boundary  
130 layers of leaves and canopy, as well as influencing storage of energy within plant organs and the soil.  
131 However, those models require complex mathematical formulations. Therefore, few 3D models have included  
132 these processes (Sellier et al., 2008; Kerzenmacher and Gardiner, 1998). The MAESPA model has to keep its  
133 principal originality and advantage (i.e. complete description of water, carbon and energy fluxes in the  
134 ecosystem at tree scale, but relatively simple description and simplifications that allow fast computation)  
135 Thus, we used the classical conductance schemes of Choudhury and Monteith (1988) to compute  $T_{air_{canopy}}$  and  
136  $V_{Pair_{canopy}}$  as a compromise that improves leaf-temperature calculations without a great increase in the  
137 model's complexity or execution time, keeping MAESPA's intermediate position between complex 3D  
138 models, and over-simplified ones.

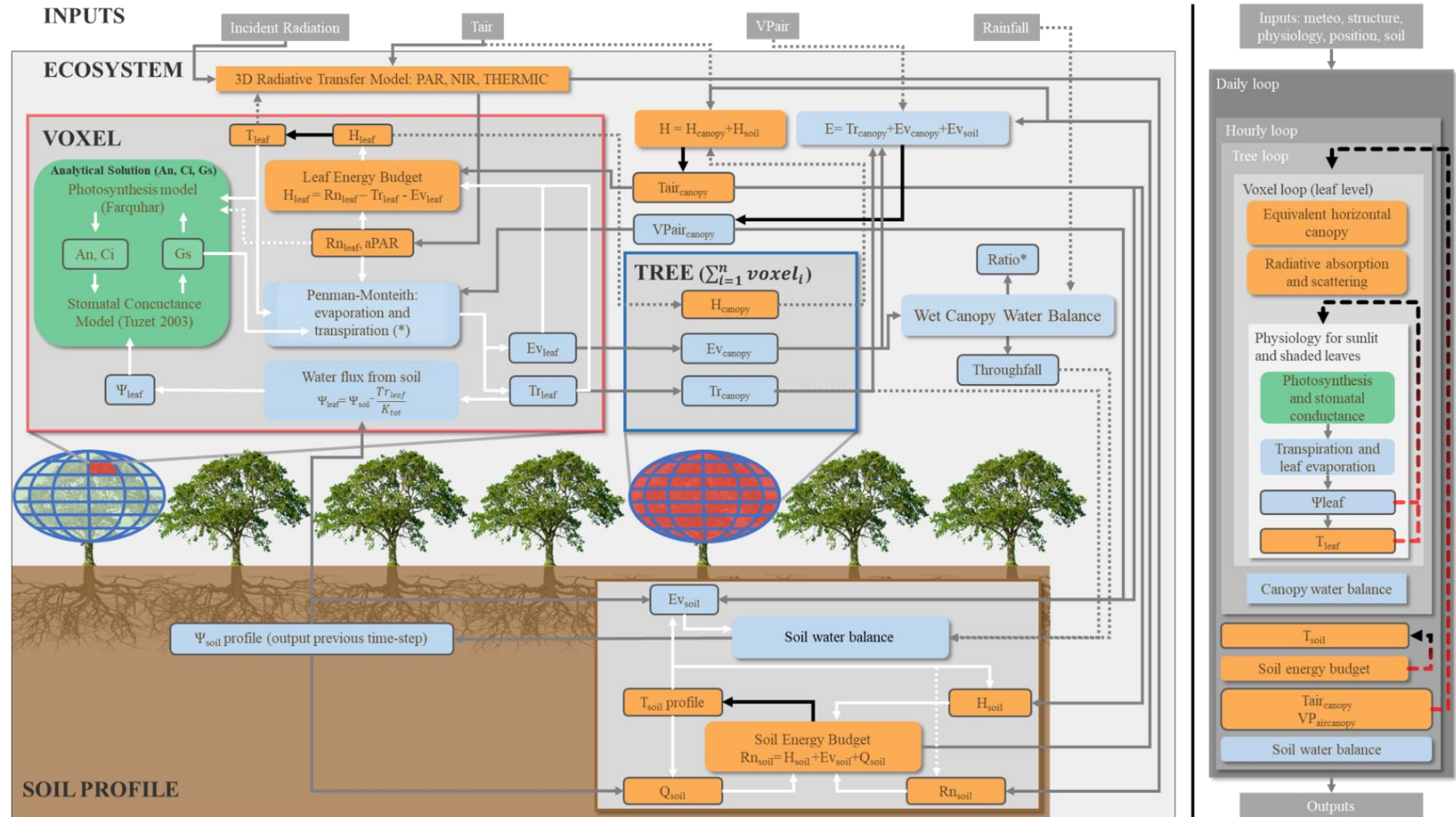
139 In summary, this paper aims to:

- 140 • Improve MAESPA through a refined representation of the canopy micro-climate (temperature and VP);
- 141 • Test the modified version of MAESPA on three perennial systems of increasing structural heterogeneity:  
142 (i) a monospecific, even-aged *Eucalyptus urophylla x grandis* plantation in Brazil; (ii) a monospecific,  
143 full-sun *Coffea* plantation, whose plants contain shoots of diverse ages due to periodic pruning and re-  
144 sprouting of *Coffea* plants; and (iii) a pluri-specific, uneven-aged, and spatially heterogeneous *Coffea*  
145 agroforestry system with tall shade trees.
- 146 • Use MAESPA to estimate energy and evapotranspiration partitioning between soil and plant layers in the  
147 simple and complex stands mentioned in the preceding point.

## 148 **2. Materials and methods**

### 149 **2.1. MAESPA model description and modifications**

150 MAESPA is a process-based ecophysiological model simulating fluxes of energy, water, and carbon in forest  
151 ecosystems at the tree and stand-scale levels at sub-daily time-steps (typically hourly or half-hourly time-  
152 step). Each tree in the ecosystem is described individually, and can have different sets of physiological and  
153 structural parameters; for instance, according to each tree's species, age, or size. MAESPA simulates the  
154 foliage light absorption, photosynthesis, soil evaporation, transpiration, and balances of water and energy.  
155 Compared to the previous version of Duursma and Medlyn (2012) and Christina et al. (2017), the version used  
156 in this study improves simulation of leaf temperatures and of foliage evaporation after rain events, as  
157 described below.



158  
 159 **Figure 9. Detailed MAESPA model workflow. Some calculations are made at the voxel scale (VOXEL, in red) before being summed for upscaling to tree level (TREE). Other**  
 160 **calculations are made directly at ecosystem level (ECOSYSTEM) such as the soil energy budget and the water balance. Voxel-scale photosynthetic module is represented in green,**  
 161 **energy modules (or variables) in orange and water-related modules (or variables) in blue. Black arrows emphasize the variables that are optimized. Linear workflow is shown on the**  
 162 **right-side, showing the three iterative computations with arrows. (\*): A ratio of dry/wet canopy is used at voxel scale for evaporation and transpiration partitioning.**

163 The initial MAESPA model calculates two largely independent energy balances: one for the foliage, and one  
164 for the soil (Figure 9). The foliage energy balance is computed at the voxel scale for each tree. Each voxel  
165 contains a given amount of leaf area within a tree, which has a set of homogeneous properties such as leaf  
166 inclination angle distribution, optical properties, photosynthetic parameters, etc. The net radiation ( $R_n$ ) of this  
167 voxel is computed from the light interception sub-modules in 3 spectral domains: the photosynthetically active  
168 radiation (PAR), near infrared (NIR) and the thermal domains. This light interception submodule takes into  
169 account the 3D representation of the stand, in which each tree is located according to its x,y,z coordinates, and  
170 characterized by its height, crown length, radius, shape (e.g. half-ellipsoids), and total leaf area. The latent  
171 heat flux of each voxel (leaf transpiration and evaporation) is computed from the Penman-Monteith equation,  
172 using  $R_n$ , stomatal and leaf to canopy air conductance, leaf temperature (set at  $T_{air_{canopy}}$  first),  $T_{air_{canopy}}$  and  
173  $V_{Pair_{canopy}}$ . Neglecting the energy storage in the leaves, each voxel's sensible-heat flux is inferred as the  
174 difference between its net radiation and its latent-heat flux. Those values of sensible-heat flux are then used to  
175 re-calculate the leaf temperatures of that voxel, based on the leaf boundary layer conductance for heat using  
176 the equations from Leuning et al. (1995). Since leaf temperature influences the voxel-scale transpiration and  
177 photosynthesis in turn, iterations are performed for each voxel until their leaf temperature converges (Figure  
178 9). Due to differences in  $R_n$  and transpiration among voxels, a gradient in leaf temperatures will exist within  
179 the canopy when the iterations have been completed.

180 For its soil energy balance, MAEPSA assumes that the stand-scale soil net radiation ( $R_{n_s}$ ) equals the sum of  
181 the stand-scale soil latent- and sensible-heat fluxes, plus the soil heat storage. The soil surface temperature is  
182 optimized to close this energy balance, using  $T_{air_{canopy}}$  and  $V_{Pair_{canopy}}$  as the drivers of sensible and latent heat  
183 fluxes (Figure 9). In turn, this energy balance influences the soil water balance, and consequently the stomatal  
184 conductance and other foliage processes.

185 In the previous version of MAESPA, the  $T_{air_{canopy}}$  and  $V_{Pair_{canopy}}$  (used in the energy balances described  
186 above) are assumed equal to  $T_{air}$  and  $V_{Pair}$  (above canopy) values, given as model inputs from measurements  
187 made in the field. When those values are measured within the canopy, close to leaves or soil, or under  
188 conditions of high turbulence, they may be valid proxies for conditions actually experienced by leaves.  
189 However, those measured values prescribed to the model usually come from measurements taken several  
190 meters above the canopy, and therefore can be either higher or lower than  $T_{air_{canopy}}$  and  $V_{Pair_{canopy}}$ . For that  
191 reason, we added in MAESPA a new computation of  $T_{air_{canopy}}$  and  $V_{Pair_{canopy}}$  based on (above canopy)  $T_{air}$   
192 and  $V_{Pair}$ , and the canopy-atmosphere aerodynamic conductance following the scheme proposed by  
193 Choudhury and Monteith (1988). For the sake of simplicity, and to limit computational time, these two  
194 variables were assumed vertically and horizontally constant within the canopy. The ecosystem-scale  
195 evapotranspiration and sensible-heat fluxes between the air within the canopy and the atmosphere were  
196 computed as:

$$\begin{cases} Tr_{canopy} = \sum_{i=1}^n Tr_{leaf,i} & (a) \\ Ev_{canopy} = \sum_{i=1}^n Ev_{leaf,i} & (b) \\ E = Ev_{soil} + Tr_{canopy} + Ev_{canopy} & (c) \end{cases} \quad (1)$$

and,

$$\begin{cases} H_{canopy} = \sum_{i=1}^n H_{leaf,i} & (a) \\ H = H_{soil} + H_{canopy} & (b) \end{cases} \quad (2)$$

197 Where  $Ev_{soil}$  and  $H_{soil}$  are the soil evaporation and sensible-heat flux between the soil and the air in the  
 198 canopy;  $Ev_{leaf,i}$ ,  $Tr_{leaf,i}$  and  $H_{leaf,i}$  are the evaporation of the wet foliage, transpiration of the dry foliage  
 199 and sensible-heat flux for the voxel  $i$  of the ecosystem composed of  $n$  voxels (see Figure 9). All units are in W  
 200  $m^{-2}$ .

201  $T_{air_{canopy}}$  and  $VP_{air_{canopy}}$  must therefore satisfy the following equality:

$$T_{air_{canopy}} = T_{air} + \left( \frac{H}{C_{P_{air}} \cdot M_{air} \cdot g_{h_{canopy}}} \right) \quad (3)$$

$$VP_{air_{canopy}} = VP_{air} + \left( \frac{E \cdot \gamma}{C_{P_{air}} \cdot M_{air} \cdot g_{h_{canopy}}} \right) \quad (4)$$

202 Where  $T_{air}$  ( $^{\circ}C$ ) and  $VP_{air}$  (Pa) are the temperature and vapor pressure of the air above the canopy,  $C_{P_{air}}$  is  
 203 the air heat capacity ( $J \text{ kg}^{-1} \text{ K}^{-1}$ ),  $M_{air}$  is the air molar mass ( $\text{Kg mol}^{-1}$ ),  $g_{h_{canopy}}$  is the aerodynamic  
 204 conductance between the canopy and the atmosphere ( $\text{mol m}^{-2} \text{ s}^{-1}$ ) computed following the equations of Van  
 205 de Griend and Van Boxel (1989), and  $\gamma$  is the psychrometric constant ( $\text{Pa K}^{-1}$ ).

206 A new iteration scheme was introduced in MAESPA, which finds the  $T_{air_{canopy}}$  ( $^{\circ}C$ ) and  $VP_{air_{canopy}}$  (Pa) which  
 207 satisfy the equations (4) and (5). Since  $T_{air_{canopy}}$  and  $VP_{air_{canopy}}$  are used in the computations of  $H_{leaf}$ ,  $Tr_{leaf}$ ,  
 208  $Ev_{leaf}$ ,  $H_{soil}$  and  $Ev_{soil}$ , and many other processes, this iteration schemes iterates over most of the processes  
 209 simulated in MAESPA (see Figure 9, right side) including the voxel-scale leaf energy budget and the soil  
 210 energy budget. Overall, leaf temperature and the water potential of each voxel, soil surface temperature (and  
 211 consequently the soil profile temperatures), and  $T_{air_{canopy}}$  and  $VP_{air_{canopy}}$  are adjusted to close the leaf and soil  
 212 budget, and consequently the ecosystem energy budget.

213 The previous version of MAESPA model computes the rainfall interception and evaporation at the ecosystem  
 214 level. The foliage intercepts rainfall, which fills a foliage bucket model: if the current foliage surface water  
 215 content ( $WatStore$ ) exceed the maximum foliage surface water content ( $WatStore_{max}$ ) which is a function of  
 216 Leaf Area Index (LAI), then the exceeding water goes to the soil as throughfall (with a possible delay). In that  
 217 version,  $WatStore$  can decrease through canopy evaporation, computed in this case at canopy scale (Duursma  
 218 and Medlyn, 2012). In the new version, wet foliage evaporation is computed at the voxel scale through the  
 219 following procedure:  $WatStore$  is distributed among leaf voxels proportionally to their leaf area ( $WatStore_i$ ).

220 The potential leaf surface water evaporation ( $Ev_{leaf,i,0}$ ), as if the leaf surface was totally wet, is computed at  
 221 voxel-scale with the same Penman-Monteith equation as used for the transpiration but with infinite stomatal  
 222 conductance ( $g_{v\infty}$ ), considering it uses the total net radiation available for the voxel ( $R_{n_{voxel}}$ ):

$$Ev_{leaf,i} = \frac{\Delta \cdot R_{n_{voxel,i}} + M_{air} \cdot c_p \cdot VPD \cdot g_{h,i}}{(\Delta + \gamma(g_{h,i}/g_{v\infty,i})) \cdot \lambda_v} \quad (5)$$

223 where  $\Delta$  is the rate of change of saturation specific humidity with air temperature and  $\lambda_v$  is the water latent-  
 224 heat of vaporization. Similarly, a potential voxel transpiration ( $Tr_{leaf,i,0}$ ) is computed as if the leaf was totally  
 225 dry, with equation (5) with the stomatal conductance and also using the total net radiation available for of the  
 226 voxel. The Rutter et al. (1971) and Chassagneux and Choisnel (1986) models, also used in Dufrêne et al.  
 227 (2005), is used afterwards to weight these potential evaporation and transpiration values by a dryness ratio  
 228 ( $ratio_{dryness}$ ) computed as the ratio of the current to maximum water stored in the voxel:

$$ratio_{dryness,i} = 1 - \frac{WatStore_i}{WatStore_{max_i}} \quad (6)$$

$$Ev_{leaf,i} = (1 - ratio_{dryness,i}) \cdot Ev_{leaf,i,0} \quad (7)$$

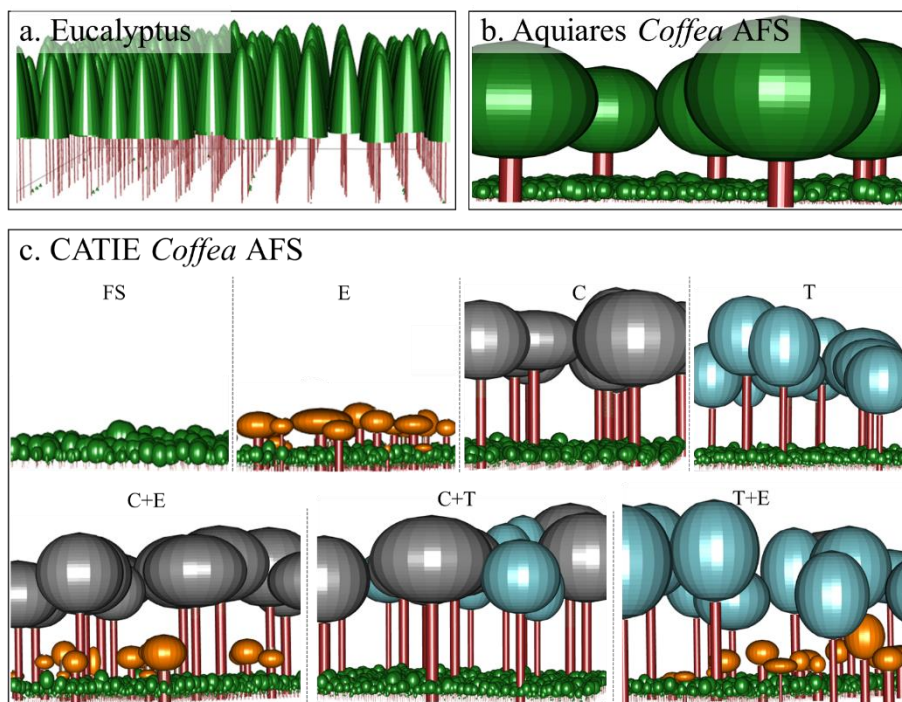
$$Tr_{leaf,i} = ratio_{dryness,i} \cdot Tr_{leaf,i,0} \quad (8)$$

229 If the computed amount of evaporated water ( $Ev_{leaf,i}$ ) is higher than the current water storage of the voxel  
 230 ( $WatStore_i$ ), the total content is evaporated, and the remaining energy is used for the transpiration. The  
 231 foliage evaporation is then summed up at the canopy scale ( $Ev_{canopy}$ ) and used for the canopy-scale water  
 232 balance as previously done in MAESPA. This modification of the MAESPA model allows to maintain closure  
 233 of the energy balance at the voxel and ecosystem level, and thereby allows a better evapotranspiration  
 234 partitioning between foliage evaporation and transpiration.

## 235 2.2. Study sites and measurements

236 Assessing the range of a model's reliability requires testing it over simple to complex systems. Three sites  
 237 were used in this study: one monospecific eucalypt stand, and two *Coffea arabica* agroforestry system (AFS)  
 238 stands (Figure 10). The first site was meant to test the new version of MAESPA for a simple, homogeneous  
 239 canopy, while the second two sites were used to test MAESPA for increasingly complex canopy structures,  
 240 starting from a simple *Coffea* plantation without shading trees (full sun) to a set of multiple conformations of  
 241 *Coffea* under shade species with various managements. The *Eucalyptus* and simple *Coffea* sites were used for  
 242 stand-scale model evaluation, while experiments on the complex *Coffea* stands were used to assess the effects  
 243 of within-stand spatial and temporal variability of light interception and leaf temperature.





244

245 **Figure 10.** Representation of tree canopies which are inputs of the MAESPA model: (a) *Eucalyptus* plantation in Brazil, (b)  
 246 *Coffea* plantations at Aquiares in Costa-Rica and (c) *Coffea* plantations at CATIE in Costa-Rica. *Eucalyptus* plantations forms  
 247 homogeneous canopies while *Coffea* AFS are more heterogeneous. Shade trees in (b) are *Erythrina poeppigiana*. Seven  
 248 plantation types are found at CATIE experimental site (c) depending upon the shade species: *Coffea* in full sun (FS, green) or  
 249 *Coffea* under shade trees *Erythrina poeppigiana* (E, orange), *Chloroleucon eurycyclum* (C, grey), *Terminalia amazonia* (T, blue),  
 250 or their mixtures (C+E ; C+T ; T+E).

### 251 2.2.1. *Eucalyptus* plantation in Itatinga, Brazil

252 The *Eucalyptus urophylla x grandis* stand has been planted at high density (2x3 m, 1666 trees ha<sup>-1</sup>) in  
 253 November 2009 at Itatinga SP area (22°58'04''S, 48°43'40''W, 750 m.a.s.l.), and managed by a commercial  
 254 company. The stand was monitored continuously in the framework of the Eucflux project  
 255 (<http://www.ipef.br/eucflux/en/>). The mean annual temperature is about 19.3°C, and the mean annual rainfall  
 256 is 1430 mm (data from 2010 to 2014). Within this stand of ~200 ha, four inventory plots of 84 trees located  
 257 around a flux-tower were chosen representative of the flux-tower footprint area. These Brazilian eucalypt  
 258 plantations are among the world's most-productive forests (Gonçalves et al., 2013). Trees are generally  
 259 harvested for their wood biomass six or seven years after planting, yielding approximately 150 t ha<sup>-1</sup> of trunk  
 260 wood dry matter. Several variables were continuously monitored at the stand scale (Table 2) using a  
 261 meteorological station and an eddy-covariance system mounted at the top of a tower. The monitored variables  
 262 included sensible-heat flux (H, W m<sup>-2</sup>), latent-heat flux (LE, W m<sup>-2</sup>), net radiation (R<sub>n</sub>, W m<sup>-2</sup>), incoming  
 263 thermal radiation (THM, W m<sup>-2</sup>) and soil water contents down to a depth of 10 m (Nouvellon et al.,  
 264 2013;Christina et al., 2017).

265

266  
267**Table 2. Measurements made on each experimental site either for input to MAESPA or for validation of its outputs. Manufacturers: [1] Campbell; [2] Gill; [3] Home-made; [4] Kipp&Zonen; [5] Licor.**

Measurement	Unit	Usage	Scale	Brazil <i>Eucalyptus</i>	Aquiaries AFS	CATIE AFS
Wind speed	m s <sup>-1</sup>	Input	Plot	WindMaster Pro <sup>[2]</sup>	WindMaster Pro <sup>[2]</sup>	CS215 <sup>[2]</sup>
Rainfall	mm	Input	Plot	ARG100 <sup>[1]</sup>	ARG100 <sup>[1]</sup>	xTE525 <sup>[1]</sup>
Air Temperature	°C	Input	Plot	HMP45 C <sup>[1]</sup>	HMP45 C <sup>[1]</sup>	CS215 <sup>[1]</sup>
Relative humidity	%	Input	Plot	HMP45 C <sup>[1]</sup>	HMP45 C <sup>[1]</sup>	CS215 <sup>[1]</sup>
RAD	W m <sup>-2</sup>	Input	Plot	?	—	—
Net Radiation	W m <sup>-2</sup>	Validation	Plot	?	NR-Lite <sup>[4]</sup>	NR-Lite <sup>[4]</sup>
Sensible-heat	W m <sup>-2</sup>	Validation	Plot	WindMaster Pro <sup>[2]</sup>	WindMaster Pro <sup>[2]</sup>	—
Latent-heat	W m <sup>-2</sup>	Validation	Plot	Li-7500 <sup>[5]</sup> & Windmaster Pro <sup>[2]</sup>	Li-7500 <sup>[5]</sup> & Windmaster Pro <sup>[2]</sup>	—
Soil water content	m <sup>3</sup> m <sup>-3</sup>	Init/Valid	Plot	CS615 <sup>[1]</sup>	CS615 <sup>[1]</sup>	CS615 <sup>[1]</sup>
Soil temperature	°C	Init/Valid	Plot	?	Thermocouples <sup>[3]</sup>	Thermocouples <sup>[3]</sup>
Light transmittance	Fraction	Validation	Plot	—	LAI 2000 <sup>[5]</sup>	Hemi-Photo
Wide-angle canopy temp.	°C	Validation	Subplot	?	IR120 <sup>[1]</sup>	IR120 <sup>[1]</sup>
Narrow-angle canopy temp.	°C	Validation	Plant	—	—	IR100 <sup>[1]</sup>
Leaf temp.	°C	Validation	Plant	—	—	Thermocouples <sup>[3]</sup>
Sap Fluxes	mmol plant <sup>-1</sup> s <sup>-1</sup>	Validation	Plant	—	TDL Granier probes <sup>[3]</sup>	—
Leaf water potential	MPa	Validation	Plant	—	PMS	—

### 268 2.2.2. *Coffea* agroforestry system in Aquiaries, Costa-Rica

269 A *Coffea arabica* (var. *Caturra*) stand planted initially at 6300 plants ha<sup>-1</sup> in the 1960's, on the slope of the  
270 Turrialba Volcano near the city of Aquiaries, Costa Rica (9°56'19''N, 83°43'46''W, 1040 m.a.s.l), has been  
271 monitored by the CoffeeFlux project ([http://www.umn-ecosols.fr/index.php/en/recherche/projets/53-coffee-](http://www.umn-ecosols.fr/index.php/en/recherche/projets/53-coffee-flux)  
272 [flux](http://www.umn-ecosols.fr/index.php/en/recherche/projets/53-coffee-flux)) since 2009. Aquiaries has a tropical humid climate (Peel et al., 2007), with a recorded mean annual  
273 temperature of 19.5°C and mean annual rainfall of 3037 mm (from 2009 to 2015). *Coffea* at Aquiaries is  
274 managed in agroforestry under free-growing *Erythrina poeppigiana* trees planted at low density (7.4 trees ha<sup>-1</sup>  
275 <sup>1</sup>), but with a canopy cover of approximately 15%. More details about the plot and instruments can be found in  
276 Gómez-Delgado et al. (2011). The portion of interest in the Aquiaries plot has an area of approximately 1.3  
277 hectares, but is surrounded by similar plantations within the 660-ha Aquiaries coffee farm. Resprouts are  
278 pruned selectively every five to six years (as soon as they become less productive), thereby creating a *Coffea*  
279 layer whose foliage is very heterogeneous horizontally (Charbonnier, 2013;Taugourdeau et al., 2014).  
280 Stand-scale values (Table 2) of sensible-heat flux (H, W m<sup>-2</sup>), latent-heat flux (LE, W m<sup>-2</sup>), net radiation (R<sub>n</sub>,  
281 W m<sup>-2</sup>), and foliage temperature ( $T_{canopy}$ , °C) were retrieved from the FLUXNET 2015 dataset (CR-AqC  
282 2009-2016). Those values have been obtained from an eddy-covariance tower between January 2011 and  
283 April 2012. In addition, sap fluxes and periodic diurnal kinetics of leaf water potential were monitored on six  
284 *Coffea* sprouts from 19 November 2014 to 31 December 2015, in order to parameterize the stomatal  
285 conductance model of Tuzet et al. (2003) that relates stomatal conductance to leaf water potential.



286 The second *Coffea* experimental trial (hereafter referred as CATIE site) was planted in 2000 in the fields of  
287 the CATIE research centre (Haggar et al., 2011) near Turrialba, Costa Rica (9°53'45"N, 83°40'04"W, 685  
288 m.a.s.l.). The *Coffea* in this experiment were planted at lower density (5000 *Coffea* plants ha<sup>-1</sup>, 1×2 m apart  
289 from each other) than at Aquiares. CATIE is a partial split-plot *Coffea* plantation experiment managed either  
290 under full sun, or under any of three species of shade trees (645 shade trees in all) which are planted above  
291 *Coffea* on a 4 × 6 m grid. The shade-tree species at CATIE are *Chloroleucon eurycyclum* (free-growing, high  
292 canopy coverage, nitrogen fixing), *Terminalia amazonia* (free-growing, high and compact canopy), and  
293 *Erythrina poeppigiana* (pruned to 3-4 m tall to optimize *Coffea* light intake during flowering and nutrient  
294 feed-back to soil). Being located less than 10 km apart, the CATIE and the Aquiares share the same tropical  
295 humid climate, but due to its lower elevation, the CATIE site has a 3.5 °C higher mean annual temperature  
296 (23°C) and a 337 mm lower mean annual rainfall with 2700 mm (Gagliardi et al., 2015).

297 The *Eucalyptus* and Aquiares sites were used for stand-scale model evaluation, while the sets of experiments  
298 at the CATIE site were used to assess the effects of within-stand spatial and temporal variability of light  
299 interception and leaf temperature. In CATIE, ten *Coffea* trees were selected at random in each subplot,  
300 yielding a total of 570 *Coffea* trees (10 trees x 19 sub-plots x 3 blocks). On each of those trees, the crown  
301 openness of the above shading layer was estimated by the Diffuse Non-Interceptance (DIFN) variable  
302 obtained from hemispherical photographs taken above each of these *Coffea* tree. This variable will be  
303 compared to the DIFN simulated by MAESPA at the same location. Leaf temperature of these *Coffea* trees  
304 were measured at three levels within the canopy (top, middle, and lower parts of the crown) with  
305 thermocouple positioned under the leaves. Tree leaves temperature (T<sub>c</sub>) was an average of these layer  
306 temperature. For practical reasons, these measurements were limited in time (15 minutes per tree). In parallel,  
307 *Coffea* canopy temperature were monitored continuously during one year on six *Coffea* trees, three in a  
308 reference full-sun plot, and three on a reference mixed *Chloroleucon eurycyclum* and *Erythrina poeppigiana*  
309 (C+E) shaded plot. For these measurements, we used IR100 thermoradiometer (Campbell Scientific) located  
310 on fixed antennas and measuring the *Coffea* at a distance of 50 cm. The antennas were equipped with  
311 complete meteorological stations. All measurements on these fixed antennas were integrated to 30 minutes  
312 time-step. The two types of measurements were complementary: the measurements made upon the 570 *Coffea*  
313 trees sample the spatial variability of *Coffea* temperature (referred as the “CATIE spatial experiment”), while  
314 the measurements of the 2×3 *Coffea* plants sample the hourly to seasonal variation of *Coffea* temperature  
315 (“CATIE temporal experiment”). All these measurements are described in detail in Soma et al. (in prep.).

### 316 **2.3. MAESPA model parameterization**

317 In the *Eucalyptus* plantations, MAESPA was fully parameterized following Christina et al. (2017). All  
318 parameters used in this version are detailed in supplementary material Table A1. Meteorological inputs  
319 included global radiation (W m<sup>-2</sup>), air temperature (°C), relative humidity (%), atmospheric pressure (Pa),

320 precipitations (mm) and incoming thermal radiation ( $\text{W m}^{-2}$ ), all measured a few meters above canopy (Table  
321 2).

322 *Coffea* plantations were simulated in MAESPA at the resprout level as in Charbonnier et al. (2013) to better  
323 account for within-plant structural heterogeneity caused by pruning. The AQUIARES site was parameterized  
324 following Charbonnier (2013) for the part concerning the light interception. LAI dynamics of *Coffea* and  
325 *Erythrina* were reported in Taugourdeau et al. (2014a). Photosynthesis parameters were obtained from  
326 Charbonnier (2013). The stomatal conductance model of Tuzet et al. (2003) was used because of its ability to  
327 link the leaf water potential with the stomatal conductance (Annexe 2, Fig. A1). The soil module was  
328 parameterized following the Van Genuchten (1980) equations using TDR measurements of soil water content  
329 at depths of up to 4 m (i.e. throughout *Coffea* entire rooting depth (Defrenet et al., 2016)). To parameterize  
330 MAESPA thermic-conductivity module, soil temperature was measured from surface to 2 m depth.  
331 Meteorological inputs were measured at a height of 24 m high and comprised PAR ( $\mu\text{mol m}^{-2} \text{s}^{-1}$ ), wind speed  
332 ( $\text{m s}^{-1}$ ), air temperature ( $^{\circ}\text{C}$ ), relative humidity (%), atmospheric pressure (Pa) and precipitation (mm). In  
333 order to estimate wind-profile parameters, wind speed was also measured continuously at 3 m, and for short  
334 periods at 5, 10, 15 and 20 m. As the incident thermal radiation was not measured, it was computed within  
335 MAESPA from air temperature and VPD by applying the Brutsaert (1975) formula for clear-sky emission and  
336 the Monteith and Unsworth (1990) correction for cloudy skies.

337 At the CATIE site, the shade-tree architecture (height of crown insertion and crown length and diameter) was  
338 extracted from rescaled orthogonal horizontal digital photographs, and their position recorded using a high-  
339 resolution Trimble Geo XT GPS. Their leaf area was computed from leaf area density (LAD) and crown  
340 volume, both of which changed with time. The maximum LAD and the leaf-angle distribution were computed  
341 from hemispherical photographs made on single trees for each species during high-LAI season. Temporal  
342 dynamics and crown volumes of those trees were inferred from photographic and visual surveys. The *Coffea*  
343 plants locations were captured as a 2x1 m grid following the *Coffea* rows that appear on the very high-  
344 resolution Pleiades satellite panchromatic image at 0.5 m resolution (Le Maire et al., 2014). The coffee sprout  
345 number, dimensions and leaf area were set according to the AQUIARES coffee site, using allometric relationships  
346 to match the measured mean height for each CATIE site management plot. Structural parameters (leaf area,  
347 number of resprouts per plant, sprout height and radius, DBH) were measured on all 6 plants in the CATIE  
348 temporal experiment, while parameters for the 570 CATIE spatial experiment were adjusted according to their  
349 measured height. *Coffea* physiology and soil parameters were assumed to be the same to those at the AQUIARES  
350 site. MAESPA's soil module was initialised for water content and temperature for each soil layer using TDR  
351 measurements (Table 2). Linear interpolation was used between soil layers for missing measurements.

## 352 2.4. Data processing

353 In the *Eucalyptus* plantation, MAESPA was run at a 15 minute time-step in order to correctly simulate the fast  
354 water flow occurring in the sandy soil after high rainfall events within reasonable computation time (Christina

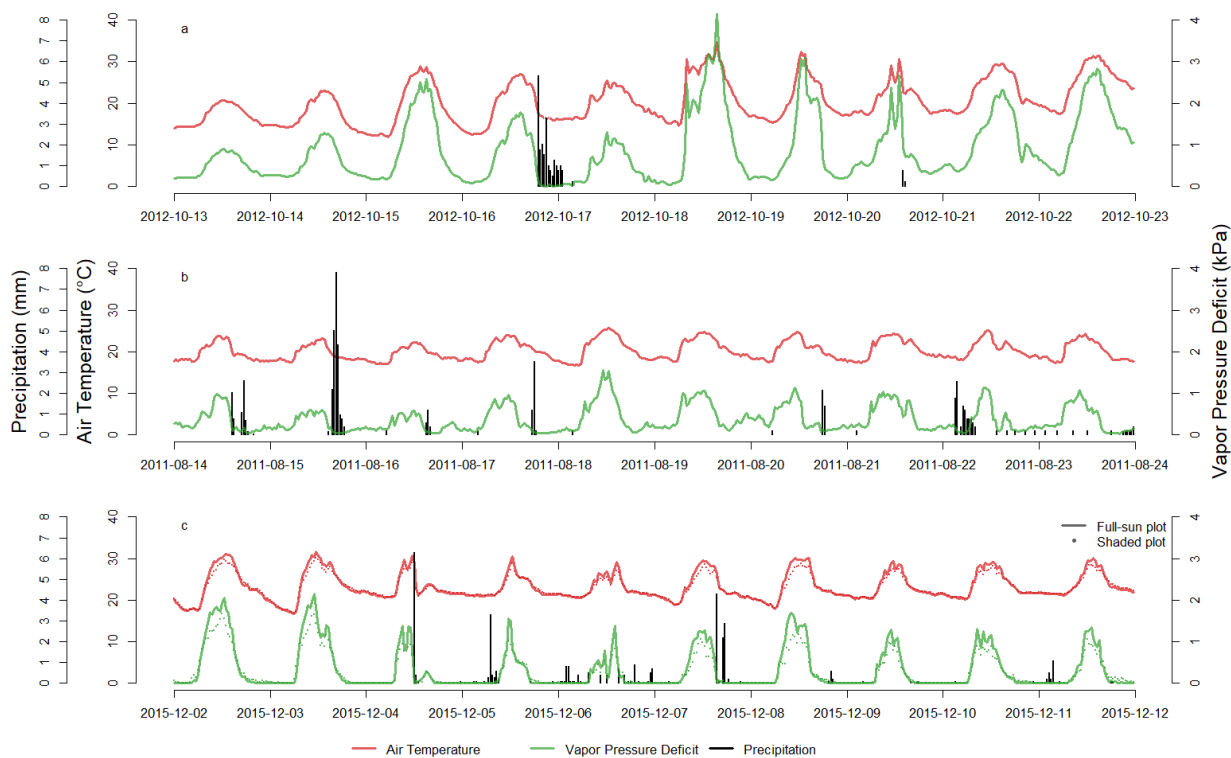
355 et al., 2017). Simulated variables were then integrated over 30-minutes for comparison with measured net  
356 radiation, latent- and sensible-heat fluxes. The simulations were carried-out throughout one year during the  
357 highest-LAI period (3<sup>rd</sup> year after plantation, 2012) at the *Eucalyptus* plantation. For the *Coffea* plantations,  
358 the MAESPA model was run at a 30 minutes time-step, since there was no such fast soil water dynamics.  
359 Simulations were performed for the year 2011 at the AQUIARES site, and for year 2015 at the CATIE site. In  
360 AQUIARES, a sub-plot containing 4176 *Coffea* sprouts that was shown to be representative of the entire stand in  
361 preliminary tests was chosen for the simulations over the entire year. In CATIE, MAESPA was run  
362 independently on each small management plot, including all the *Coffea* sprouts of the small plots (~1400  
363 sprouts) and all shade trees which can influence the incoming light in the small plot (therefore also the shade  
364 trees outside the small plot). Tree-scale MAESPA outputs were then processed using R (R Core Team, 2016).

### 365 **3. Results**

#### 366 **3.1. *Eucalyptus* plantation – homogeneous stand**

367 A 10 days' time-series measurement period was chosen for output assessment according to the variability of  
368 the meteorological conditions, with high and low values of air temperature and vapor pressure deficit as well  
369 as rain events followed by at least one day without rain (Figure 11).

370 The daily variations of the simulated net radiation during this short period followed measured variations  
371 closely (Figure 12.1.a). Half-hourly values were in agreement with measurements throughout the year (Figure  
372 12.1.b, RMSE= 31.2 W m<sup>-2</sup>). Net radiation simulation error was lowest during night time and although  
373 MAESPA frequently overestimated net radiation just after sunrise (c.a. 7:15 am), the error was approximately  
374 homogeneous during the day. Simulated latent-heat fluxes were also in good agreement with the diurnal time-  
375 course of measurements (Figure 12.2.a) for low to high values during the ten-day period. Throughout the year,  
376 half-hourly values were simulated well but the model systematically underestimated the rare highest measured  
377 values (c.a.  $\geq 700$  W m<sup>-2</sup>), which probably are measurement noise or error.

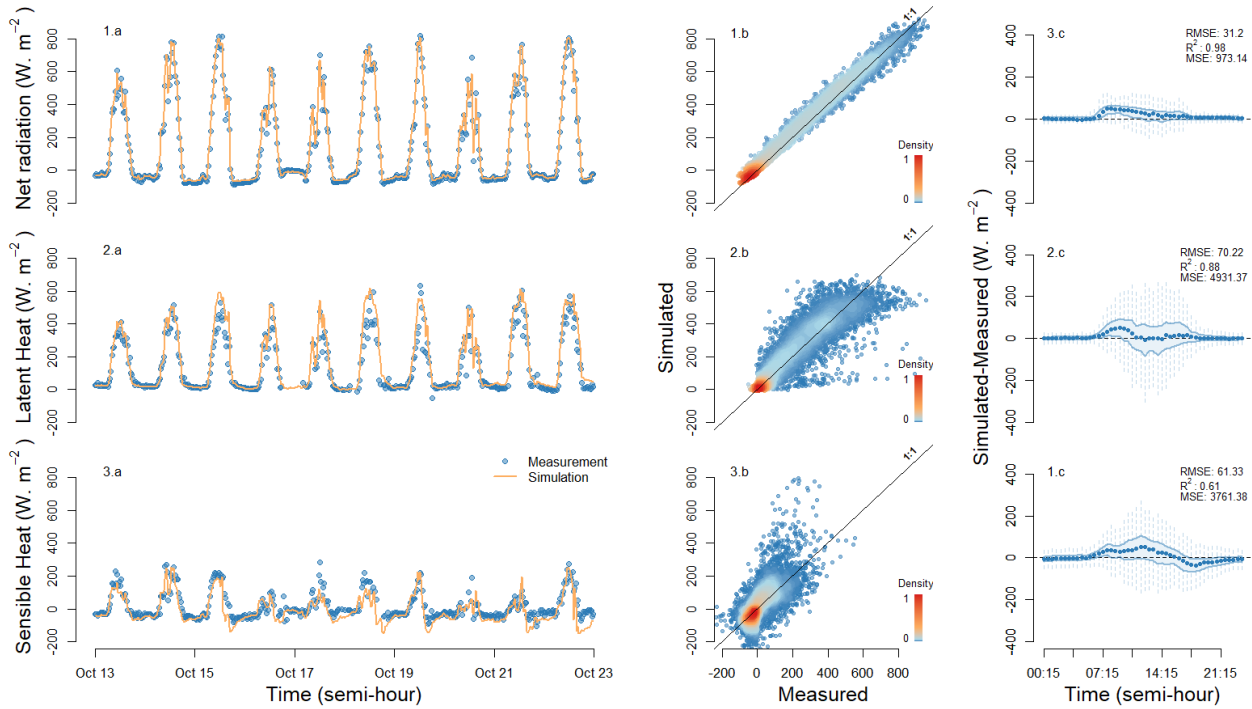


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**Figure 11. Half-hour precipitation, air temperature and Vapor Pressure Deficit measured above forest canopy during the ten-day period used for MAESPA model simulations presented in Figure 12, Figure 15 and Figure 17, for (a) *Eucalyptus* plantation in Brazil, (b) *Coffea* plantations at Aquiares in Costa-Rica and (c) *Coffea* plantations at CATIE site in Costa-Rica.**

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The RMSE ( $70.2 \text{ W m}^{-2}$ ) was twice as high as for  $R_n$ , with low median bias during the day except at sunrise when the model often overestimated the fluxes. Errors during the day increased in proportion with the values, but generally stayed within a  $\pm 70 \text{ W m}^{-2}$  range, with rare extreme values. The diurnal time-course of sensible-heat fluxes followed measured values during the 10-day period. Although the RMSE values remained quite low (Figure 12.3.b, i.e.  $61.3 \text{ W m}^{-2}$ ) compared to that for latent-heat fluxes, this error was relatively high compared to the mean values. Indeed, sensible-heat fluxes in this ecosystem were lower than latent-heat flux. On average, the model overestimated sensible-heat fluxes slightly from sunrise to 16:00, after which it underestimated them slightly. In terms of agreement between simulated and measured values, the new version of the model showed an improvement of 1% for  $R_n$ , 8% for LE and 10% for H relative to the measurements compared to the same version that did not calculate  $T_{\text{air}_{\text{canopy}}}$  or  $V_{\text{Pair}_{\text{canopy}}}$  (data not shown).



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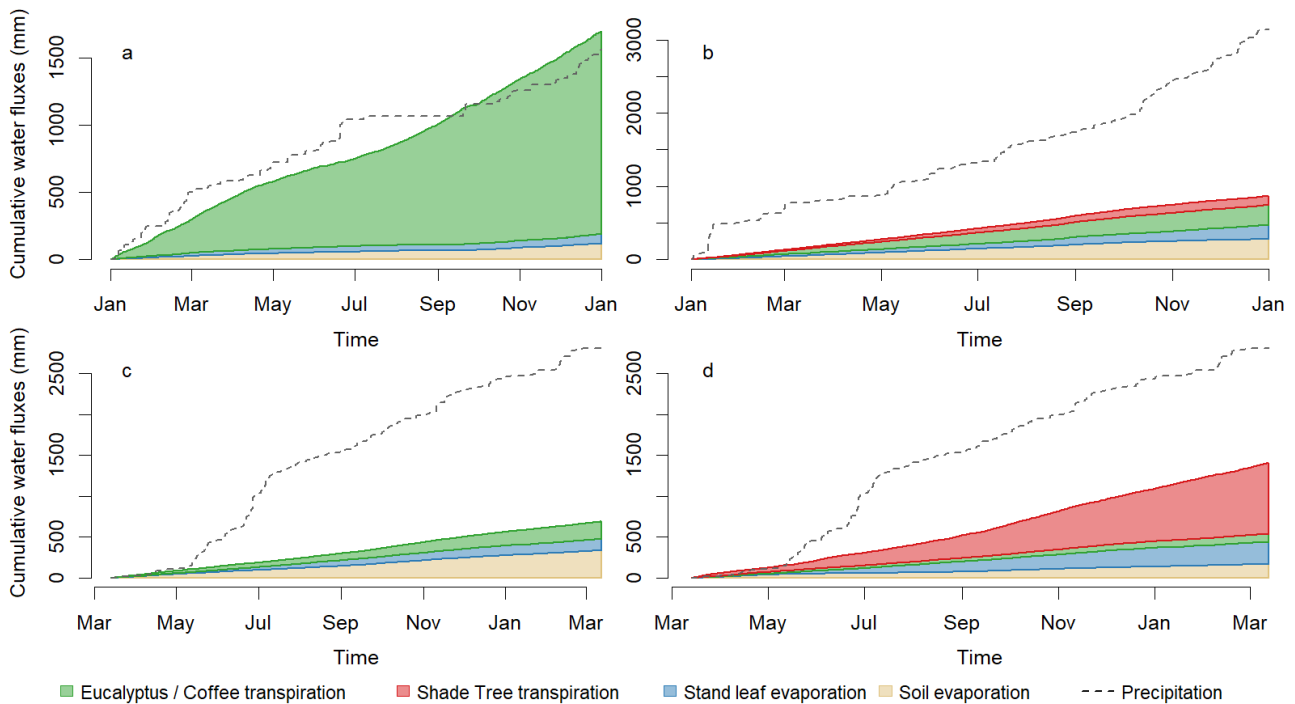
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Figure 12. Measured and modelled net radiation (top), latent heat (middle) and sensible heat (bottom) fluxes in the *Eucalyptus* plantation in Brazil, at a half-hourly time-scale. a) diurnal time courses over 10 days (meteorology presented in Figure 11); b) Yearly scatter plots of all half-hourly values in 2012. Colors represent density of the points; c) Minimal boxplots (Tufté, 1983) of the diurnal time course of residuals (simulated - Measured) in 2012, dots indicate the median, horizontal lines represents the first and third quartile, and the end of vertical lines indicates minimum and maximum without outliers.



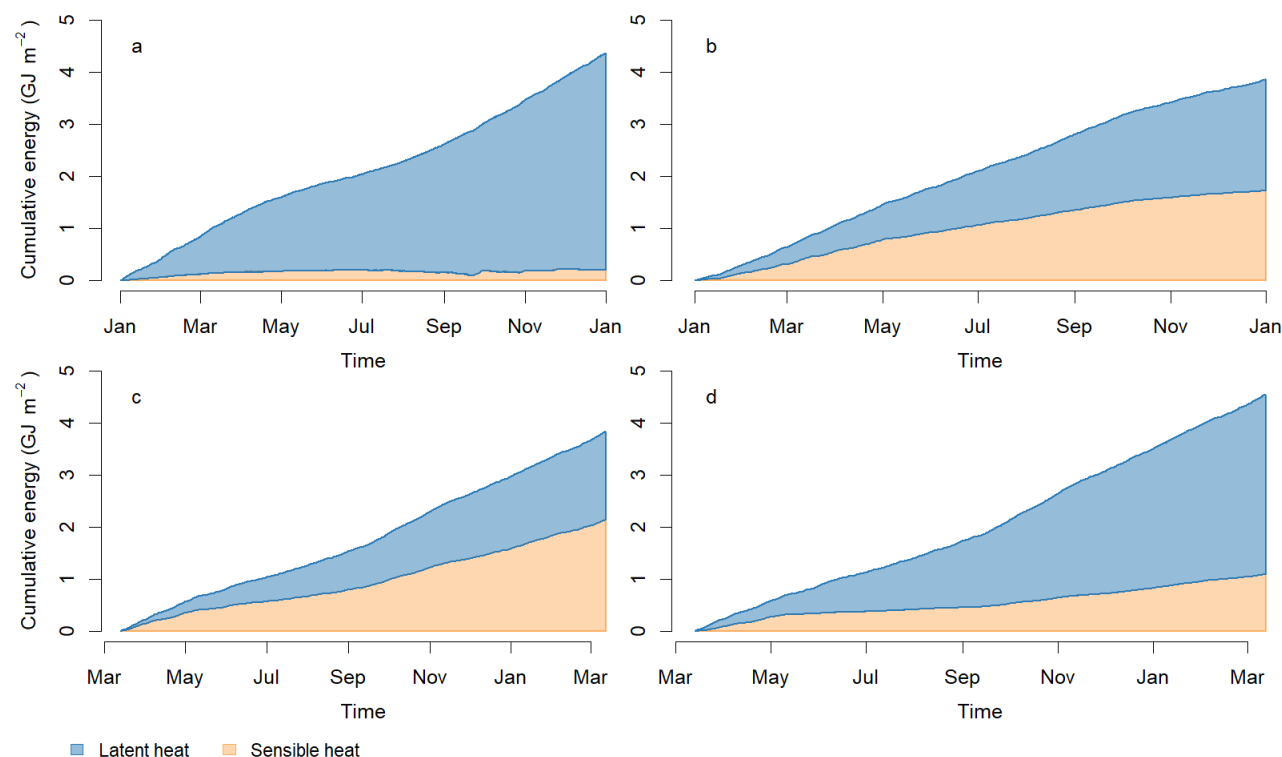
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Figure 13. Cumulated simulated evapotranspiration partitioning and cumulated precipitation for the a) *Eucalyptus* stand (year 2012), b) *Coffea Aquiares* AFS plantation with *E. poeppigiana* (year 2011), c) *Coffea* CATIE full-sun management (one year starting the 2015-03-13) and d) *Coffea* CATIE grown under C+E shade trees (same period than c).



402

403 **Figure 14. Cumulated simulated energy partitioning for the a) *Eucalyptus* stand (year 2012), b) *Coffea* Aquiares AFS**  
 404 **plantation with *E. poeppigiana* (year 2011), c) *Coffea* CATIE full-sun management (one year starting the 2015-03-13) and d)**  
 405 ***Coffea* CATIE grown under C+E shade trees (same period than c)). Cumulated soil heat storage is not shown because it**  
 406 **remained close to 0.**

407 Simulations showed that evapotranspiration partitioning for the *Eucalyptus* plantation during the year 2012  
 408 was strongly dominated by the transpiration component (Figure 13.a). Indeed, the annual *Eucalyptus*  
 409 transpiration (c.a. 1509 mm) represented 89% of the total simulated AET (c.a. 1697 mm). Soil evaporation  
 410 and leaf evaporation accounted for just 7% and 4% of the total AET, respectively. In this ecosystem, and  
 411 during that year, AET was higher than the total precipitation (c.a. 1562 mm). During the dry season, between  
 412 August and October, the transpiration flux remained high (451 mm), while soil and leaf evaporation were  
 413 close to zero (23 mm and 10 mm respectively, compared to 189 mm of rainfall).

414 In the ecosystem energy balance (Figure 14.a), latent energy was the major component by far. Its contribution  
 415 was 95% of the total net radiation of that year, while it was only 5% for the sensible flux. Negative sensible-  
 416 heat flux at the end of afternoon (after 16:00) and during the night compensated almost entirely for the  
 417 positive diurnal fluxes.

### 418 3.2. Aquiares *Coffea* agroforestry system –heterogeneous plot

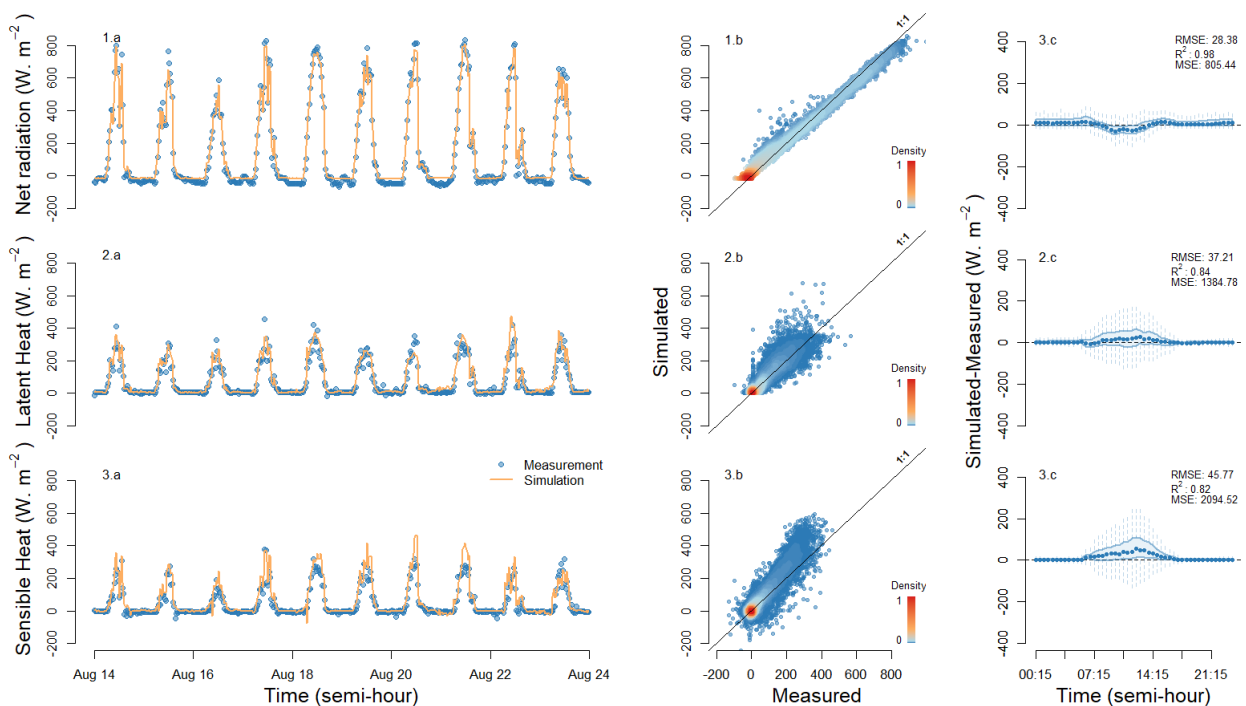
419 MAESPA simulations of all three energy-fluxes variables for the Aquiares *Coffea* agroforestry plantation  
 420 followed measured values during the modelled ten-day period (Figure 15.a). The net radiation fluxes were  
 421 simulated correctly at a half-hour time-step during the entire year of 2011, with a RMSE of 28.4 W m<sup>-2</sup>  
 422 (Figure 15 1.b-c). High values around noon were slightly overestimated. Latent-heat flux simulations were

423 also realistic, as the general trend was close to the identity function ( $R^2= 0.88$ ,  $MSE= 1.42$ , Figure 15 2.b), and  
 424 the median of the residuals remained close to zero throughout the day (Figure 15.2.c). However, results  
 425 showed heteroscedasticity, although for only a few half-hour observations during that year. Sensible-heat  
 426 fluxes were overestimated for the highest measured values ( $>300 \text{ W m}^{-2}$ ), the average error was  $120.8 \text{ W m}^{-2}$ .  
 427 This error had a clear diurnal pattern, which was correlated with an increase in the incoming and net radiation  
 428 fluxes (Figure 15.3.c). It should be noted that the measured fluxes did not show closure of energy balance in  
 429 AQUIARES. Indeed, the yearly cumulative net radiation was 17% higher than the yearly sum of the cumulative  
 430 latent- and sensible-heat fluxes.

431 According to the model, the total annual AET of AQUIARES AFS for the year 2011 was 870 mm (Figure 13.b),  
 432 i.e. 27.7% of the annual precipitation (c.a. 3144 mm). The transpiration of *Coffea* and shade trees represented  
 433 45.7% of the AET, with 14.3% coming from the shade trees and 31.4% from the *Coffea* plants. Soil  
 434 evaporation represented 32.5% of the total AET, while wet-foliage evaporation from shade trees + *Coffea*  
 435 represented 21.8%.

436 Within the AQUIARES site's *Coffea* agroforestry system, total net radiation was partitioned relatively evenly  
 437 between the latent-heat flux (with 55% of the total net radiation) and sensible-heat flux (with 45% of  $R_n$ ,  
 438 Figure 14.b).

439



440

441 **Figure 15.** Measured and modelled net radiation (top), latent heat (middle) and sensible heat (bottom) fluxes in the AQUIARES  
 442 *Coffea* agroforestry plantation in Costa Rica, at a half-hourly time-scale. a) diurnal time courses over 10 days (meteorology  
 443 presented in Figure 11); b) Yearly scatter plots of all half-hourly values in 2011. Colors represent density of the points; c)  
 444 Minimal boxplots (Tufté, 1983) of the diurnal time course of residuals (simulated - Measured) in 2012, dots indicate the  
 445 median, horizontal lines represents the first and third quartile, and the end of vertical lines indicates minimum and maximum  
 446 without outliers.

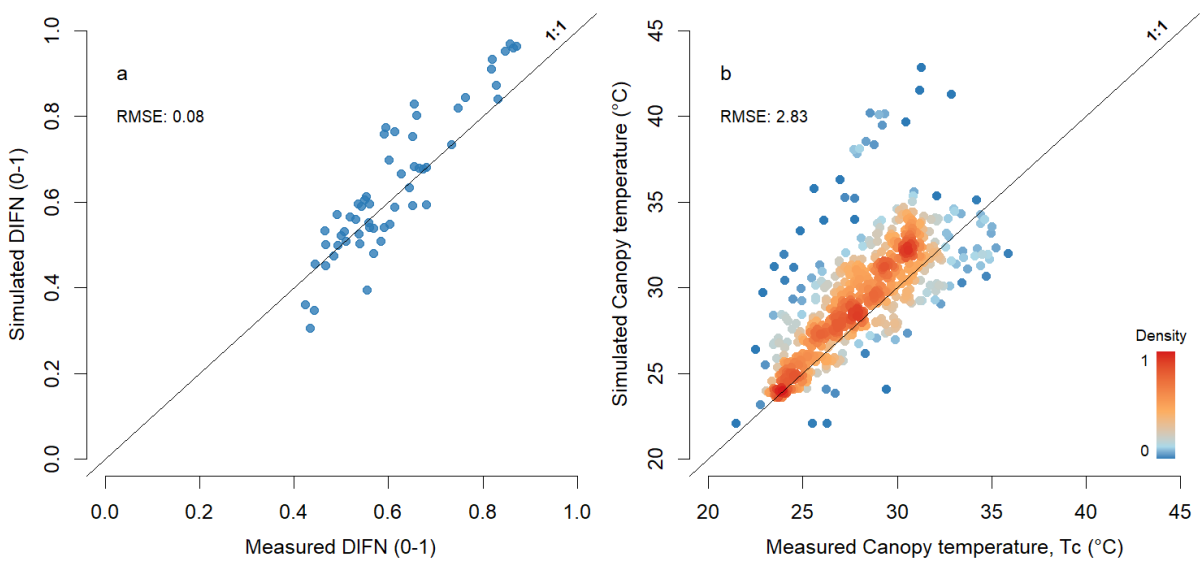
447 The CATIE site had an annual precipitation of 2816 mm during the study period. Modelled AET was about  
448 689 mm (24.5% of the rainfall) for the full sun stand, compared to 1404.8 mm (49.9% of the rainfall) for the  
449 shaded stand (Figure 13 c-d). In the full-sun stand, the soil evaporation, wet-foliage evaporation, and  
450 transpiration respectively contributed 48.8%, 19.8% and 31.4% of AET, versus 12.3%, 18.8% and 68.9% of  
451 AET for the shaded stand. However, the *Coffea* transpiration in the shaded stand represented only 7.2% of the  
452 total AET while the two shade tree species contributed 61.7%. The mean total LAI during the six-month  
453 period was 3.6 m<sup>2</sup> m<sup>-2</sup> (min. 2.2, max. 4.4) in full sun and 6.6 m<sup>2</sup> m<sup>-2</sup> (min. at 2.4, max. 8.4) in the shaded plot  
454 (for shade trees + *Coffea*). The *Coffea* LAI in the shaded plot was the same as in full sun.  
455 Full-sun and shaded plots differed greatly in their partitioning of AET among plants, wet-foliage, and soil  
456 evaporation. Soil evaporation in the shaded plot was reduced by half compared to full sun plot, but wet-foliage  
457 evaporation was doubled because of the higher LAI (shade tree + *Coffea*). *Coffea* transpiration was reduced by  
458 a factor of two under shade trees as compared to full sun, but the shade-tree transpiration more than  
459 compensated for this reduction. Finally, the total transpiration was 752 mm lower in full sun than in the  
460 shaded agroforestry plot. Overall, the shade plot's AET was twice that of the full sun plot.  
461 In the CATIE full-sun plantation, latent- and sensible-heat fluxes represented 44% and 56% of the available  
462 energy (total net radiation), respectively, versus 76% and 24% in the CATIE's shaded AFS (Figure 14 c-d).  
463 Sensible-heat flux was lower in the shaded plot, but latent-heat flux was higher.

### 464 3.3. Shading effect on canopy temperature– Tree scale

465 Simulated DIFN of shade trees were compared to values that had been measured at the CATIE site in full sun,  
466 and along a shading gradient within the agroforestry trial plot (Figure 16.a). Simulated DIFNs were unbiased  
467 (*i.e.* most of the data points fell around the identity function) and their RMSE was small, at 0.08. In contrast,  
468 RMSE of simulated *Coffea* canopy temperature measured on the CATIE spatial experiment was large, at 2.8  
469 °C (Figure 16.b), but only few values were largely overestimated by the model.  
470 MAESPA canopy-temperature simulations on three *Coffea* plants under shaded and full-sun management  
471 were compared to one year of continuous measurements in the CATIE temporal experiment, using IR100  
472 thermoradiometer (Figure 17). The model accurately simulated the diurnal time course during the ten-day  
473 example period under full sun and shaded management (RMSE = 1.7 and 1.4 °C respectively, Figure 17 a).  
474 However, the lowest leaf temperature (<25°C) were underestimated frequently (<25 °C, Figure 17 b). This  
475 phenomenon was confirmed by inspection of the residuals, which showed the largest overestimation in the  
476 morning, followed by some underestimation in the afternoon or just before sunset (Figure 17 c). These  
477 discrepancies may arise because the simulation overestimates both the rate of leaf heating in the morning, and  
478 the rate of leaf cooling at day's end, which is shown on the Tleaf-Tair average daily variations. There is a time  
479 shift in the leaf heating and cooling during the day, compared with measurements. However, the amplitude of  
480 the variation and the variability are similar. Plantations under shade trees showed a simulated increase in  
481 Tleaf-Tair, in the morning, which was not observed in the measurements.

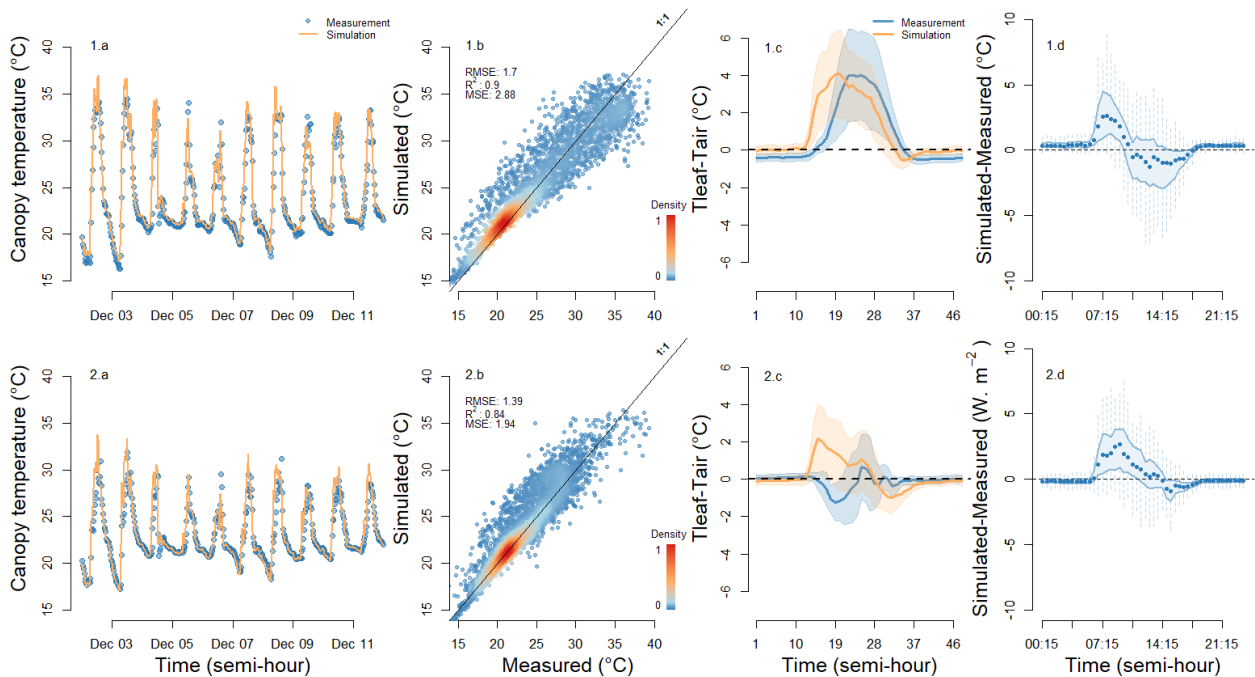


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484 **Figure 16. Measured and modelled a) Diffuse Non-Interceptance of the shade trees at the CATIE *Coffea* agroforestry**  
 485 **plantation site, averaged by treatment, and b) canopy temperature ( $T_c$ ) in the same site (color scale represents the point**  
 486 **density).**



487

488 **Figure 17. Measured and modelled canopy temperature averaged between three plants in CATIE site *Coffea* agroforestry**  
 489 **plantation (Costa Rica) under 1) full-sun (top) or 2) shaded management (bottom); a) diurnal time courses over 10 days**  
 490 **(meteorology presented in Figure 11); b) Yearly scatter plots of all half-hourly values between 13-03-2015 and 12-03-2016).**  
 491 **Colors represent density of the points; c) Diurnal time course of the simulated and measured difference between the leaf and the**  
 492 **air temperature; d) Minimal boxplots (Tufté, 1983) of the diurnal time course of residuals (simulated - Measured) in 2012,**  
 493 **dots indicate the median, horizontal lines represents the first and third quartile, and the end of vertical lines indicates**  
 494 **minimum and maximum without outliers.**

## 495 4. Discussion

### 496 4.1. Energy flux simulation and partitioning between H and LE

497 The evaluation of the modified MAESPA model demonstrated its ability to provide accurate simulations of  
498 energy fluxes for both the *Eucalyptus* and the *Coffea* plantations, thus indicating that the model is sufficiently  
499 generic to be applied to agricultural systems of contrasting levels of complexity. The model's small over-  
500 estimation of the net radiation just after sunrise in the *Eucalyptus* plantation led to a slight discrepancy for  
501 both latent- and sensible-energy fluxes, emphasizing that an accurate simulation of the net radiation is critical,  
502 and that careful attention must be given to the parameterization of the model for light interception, scattering  
503 and emissivity. If possible, all incoming radiations (global and thermal) should be forced in the model. Here,  
504 the incoming thermal radiation was forced for eucalypt but simulated for *Coffea*, leading to a higher night-  
505 time error for the *Coffea* (Figure 15), and probably to greater day-time error as well. Other errors may arise  
506 through insufficient precision or an excessive simplification of some processes such as the simplified  
507 aerodynamic conductance module, the assumption that  $T_{air_{canopy}}$  and  $V_{Pair_{canopy}}$  are constant within the  
508 canopy, the lack of energy storage in the plants, the uniform water storage on leaf surface after rainfall events  
509 (in reality, higher leaves are filled first) or through measurement error for the plant structure. A data-model  
510 mismatch can also arise from errors in the data. Although open-path eddy covariance has been used for several  
511 decades and is considered to be an accurate method for measuring water and carbon fluxes (Larsen et al.,  
512 2016), it can present some problems, especially during unstable conditions (Stoy et al., 2013). For example,  
513 MAESPA tended to over-estimate fluxes just after sunrise, which may be partly explained by lack of  
514 measured energy balance closure, which may happen in early morning as found in Stoy et al. (2013). Also,  
515 Haslwanter et al. (2009) showed that latent-heat flux measurements made by open and closed-path eddy-  
516 covariance systems differed by  $16.7 \text{ W m}^{-2}$ . Similarly, Mauder et al. (2013) found that random error in eddy-  
517 covariance systems is typically 20–30% for most turbulent fluxes. Therefore, MAESPA simulation errors fall  
518 within the range of the measurement's stochastic errors.

519 Another point to be considered is the voxel size and the lack of tree branches (shade trees and *Eucalyptus*) and  
520 *Coffea* woody elements in the model. Indeed, Widlowski et al. (2014) compared the effects of different  
521 methods for approximating tree architecture (from exact representation, to voxels of different sizes, to a  
522 single ellipsoidal shape) on the simulated bidirectional reflectance factors (BRFs). Widlowski et al. (2014)  
523 found that the simulation bias (especially for NIR) not only increased with voxel size (see their Table 4) but  
524 also increased dramatically as woody elements were represented more abstractly. In our study, the average  
525 maximum voxel size (i.e. at the centre of the crown) in AQUIARES was 30 cm for *Coffea* plants and as large as  
526 c.a. 4 m for shade trees. Although *Coffea* voxel sizes were small enough, their woody part was omitted,  
527 possibly leading to high uncertainty in NIR.

528 Nonetheless, the model represented satisfactorily the sub-hourly dynamics of fluxes of the two ecosystems  
529 throughout the entire year. The new iterative scheme for computation of  $T_{air_{canopy}}$  and  $V_{Pair_{canopy}}$  improved the

530 energy and water balances notably. The model can simulate very contrasted plots realistically, such as the  
531 *Eucalyptus* plantations (in which most of the outgoing energy flux takes the form of latent- rather than  
532 sensible-heat), and the complex heterogeneous *Coffea* agroforestry systems, which has a more equal  
533 partitioning between sensible- and latent-heat fluxes.

#### 534 **4.2. Evapotranspiration and energy partitioning between trees and understorey**

535 As the comparison of the simulated fluxes against measurements yielded good results over a full year, the  
536 model was further used to estimate the partition of the evapotranspiration and the energy between their main  
537 components. Results showed that total AET of the *Eucalyptus* plantation was higher than the total  
538 precipitations in 2012 (3<sup>rd</sup> year of the rotation). This phenomenon happens because the plantation transformed  
539 almost all incoming radiant energy into latent-heat flux (Figure 14), particularly plant transpiration during the  
540 dry season from October until the end of the year. Therefore, *Eucalyptus* transpired part of the soil water that  
541 had been stored previously (Christina et al., 2017). In contrast, there was relatively little evaporation from the  
542 soil. This can be explained by a relatively fast-drying soil surface; the litter has a low water retention potential,  
543 and the sandy soil has a high water conductivity, which tends to drain the water down before it could  
544 evaporates (Christina et al., 2017). It must be noted that the year of simulation presented the highest LAI of  
545 the entire *Eucalyptus* rotation (3<sup>rd</sup> year), meaning the transpiration rate was at its maximum. The significance  
546 of the soil characteristics and the high LAI on this year is that much of the precipitation that fell upon the  
547 modelled plot during the rainy season remained below ground for months before being uptaken by roots  
548 during the dry season, then transpired back into the atmosphere. MAESPA simulated accurately that lag effect  
549 through the soil water balance, and the high fraction of energy emission and evapotranspiration occurring as  
550 plant transpiration. The modelled precipitation interception of 4.5% was in agreement with values of about 5-  
551 6% measured previously at the same site (Maquere, 2008), as well as the 8% interception measured in similar  
552 studies in Congo (Laclau et al., 2005), and the 4% measured in South Africa (Dye, 1996), all on *Eucalyptus*  
553 plantations.

554 AET partitioning by the model for the Aquiares *Coffea* system estimated that AET was 28% of total rainfall.  
555 AET was considerably less than rainfall throughout the year, meaning the system was never limited by water  
556 availability. Neither was the CATIE site, even in plots with high densities of shade trees over *Coffea* plants.  
557 Furthermore, shaded *Coffea* plants at the CATIE site transpired only half as much as those grown there in full  
558 sun, even though the shaded plot's AET was nearly double that of the full-sun plot. Indeed, the transpiration  
559 of the shade trees transformed more energy into latent-heat than sensible-heat (Figure 14), thereby changing  
560 the microclimate within the *Coffea* canopy to a cooler, more-humid one with less-intense radiation. As a  
561 result, the *Coffea* leaf temperature and transpiration were reduced.

562 Due to the lack of measurements, it is more difficult to validate the AET partitioning between canopy layers  
563 than to validate the energy balance partitioning between H and LE. Nonetheless, the simulated rainfall  
564 interception was within the range of the measurement made on a shaded *Coffea* plantation of central Veracruz,

565 Mexico by Holwerda et al. (2013), who found a 7% interception (cf. 6% in our study) during a seven-month  
566 period, with an approximate uncertainty of 43%. Our simulations of total AET and total transpiration were  
567 also in agreement with several studies that compared different *Coffea* plantations and AET partitioning  
568 methods, such as eddy-covariance, and throughfall measurements presented in Gómez-Delgado et al. (2011)  
569 for the same Aquiares site, and others from Holwerda et al. (2013).

570 Our results show that the two management practices at the CATIE site (*Coffea* in full sun, or shaded by C+E)  
571 had a relatively similar leaf + soil evaporation because the leaf evaporation doubled in the shaded plot due to a  
572 higher LAI, while the soil evaporation halved because of shading. LAI's effect (via shade-tree density) upon  
573 the partitioning between green water (evapotranspiration) and blue water (infiltration, aquifer recharge,  
574 streamflow) has already been stressed by Taugourdeau et al. (2014) in the same region. The partitioning can  
575 affect water management dramatically at regional scale because of its influence upon the extent to which  
576 rainfall recycles back into the atmosphere, as opposed to entering soil water stocks. Those results would have  
577 been difficult to infer without the help of a 3D model, because the particularly complex conditions of  
578 agroforestry systems are difficult to measure due to the high spatial heterogeneity, the complex species  
579 arrangements, and the often-asynchronous species phenology. Hence, another potential application for the  
580 MAESPA model is to use it for management optimisation. Indeed, using simple *Coffea* suitability models, it  
581 has often been forecast that yields of *Coffea arabica* will decrease under climate change because of *Coffea*  
582 high sensitivity to rising temperature (Bunn et al., 2015; Davis et al., 2012; Moat et al., 2017). However, we  
583 caution that *Coffea* suitability models do not yet take the compensatory effects of rising atmospheric CO<sub>2</sub> on  
584 photosynthesis into account so far (Rodrigues et al., 2016b). Moreover, the possibility of adapting  
585 management practices is overlooked: our results show that agroforestry management has the potential to  
586 reduce *Coffea* leaf temperatures significantly while simultaneously reducing transpiration, at least in the  
587 absence of water stress (see Figure 13 and Figure 17).

588 The model can also be used for energy partitioning, which is helpful for evapotranspiration control,  
589 assessment of climate-change impacts, and calibration of surface temperatures for satellite-based models. The  
590 method used most commonly at present for energy partitioning is the application of the Penman-Monteith  
591 equation to estimate evapotranspiration; however, this equation does not account for spatial heterogeneity in  
592 the vertical or horizontal directions. Hence, MAESPA could be used to compute metamodels (simple  
593 empirical functions derived from complete MAESPA simulations in a range of conditions) for each type of  
594 forest or management, and integrated at larger spatial scales while drastically reducing computation time, as in  
595 Christina et al. (2016) or in Marie et al. (2014).

### 596 **4.3. Canopy light interception and temperature**

597 It is important to simulate the leaf temperatures realistically because of their central role in the initiation and  
598 kinetics of several biological processes, including phenology, photosynthesis, transpiration, and autotrophic  
599 respiration. Indeed, leaf temperatures results from leaf evaporation and sensible fluxes, which in turn interact

600 with the surrounding microclimate. Compared to any other ecosystem component, the leaves have a large  
601 capacity to dissipate energy via transpiration. Thus, the difference between the air and leaf temperatures can  
602 be a good proxy for hydric stress and plant health (Chaerle and Van Der Straeten, 2001).

603 The model simulated DIFN correctly (RMSE of 0.08%). The remaining error was similar to those present in  
604 results from other studies that used MAESPA : le Maire et al. (2013), Charbonnier et al. (2013), and Christina  
605 et al. (2015). Modelled leaf-temperature trends in the CATIE spatial experiment were satisfactory overall  
606 (Figure 16.b), but presented larger errors (RMSE= 2.83°C) than in the CATIE temporal experiment (RMSE=  
607 1.4-1.7°C, Figure 17). This difference was expected because the CATIE temporal experiment was better  
608 parameterized for the target *Coffea* plants location, leaf areas, heights, and surroundings. In addition, the 30-  
609 minutes integration time in simulations of the CATIE spatial experiment didn't match the 15-minutes  
610 integration time of the measurements. Furthermore, experimental results conducted on the same site on shaded  
611 plot showed differences of up to 1.9 °C between daily averaged thermocouple measurements of foliage  
612 temperatures, and those from IR100. Several effects can lead to such differences, mainly because  
613 thermocouple measurements have multiple potential sources of error (e.g., radiative and conductive heat  
614 exchange), especially when leaf-to-air temperature difference is large (Pieters and Schurer, 1973). Also,  
615 thermocouples measure temperature at only a single point on a leaf, within which the temperature might vary  
616 by several degrees (Leigh et al., 2017; Miller, 1967). We also note that our sampling method, which used only  
617 three thermocouples per *Coffea* crown, may have been inadequate to capture the strong temperature variability  
618 therein, or to provide a good approximation of the crown's average temperature (Miller, 1971). The IR100  
619 thermoradiometer integrate the leaves temperature on a much larger footprint (approximately 60 cm<sup>2</sup>) but the  
620 location of the measure in the crown may integrate leaves at different height within the crown, and even  
621 eventually the soil. These aspects of temperature measurements are detailed in Soma et al. (in prep.) and Soma  
622 (2015).

623 In our simulations, the canopy heated faster than in reality during the morning (Figure 17.a), and cooled faster  
624 at the end of the day. This discrepancy probably results from the model's assumption that the biomass (leaves  
625 and trunk) neither stores nor releases thermal energy, and because the dew latent-heat stored on the surface of  
626 the woody elements was not represented in the model. Thus, the model does not reproduce the biomass's  
627 "buffer effect" upon temperature change, and make the model predicts well the amplitude but not the phase of  
628 the leaf temperatures throughout the day. This characteristic of the model may have had a substantial effect  
629 upon our simulated leaves and canopy air temperature because woody elements represented a relatively high  
630 proportion of biomass in all sites, especially in the *Coffea* plantations of the shaded plot in CATIE which  
631 showed an increase in Tleaf-Tair in the morning that was not observed. In support of this idea, we note that in  
632 a study by Kobayashi et al. (2012), energy storage in woody elements accounted for 12% of all daytime  
633 energy fluxes. Also, to maintain a balance between simplicity and accuracy, the MAESPA model was  
634 developed using simplified aerodynamic conductance at canopy and voxel scales via a simple wind profile,  
635 plus average plot-level values of Tair<sub>canopy</sub> and VPair<sub>canopy</sub>. Aerodynamic conductance is probably the major

636 issue now for accurate simulations during non-turbulent time-steps because it affects both sensible- and latent-  
637 heat fluxes strongly, thereby influencing energy balances and, ultimately, leaf temperatures. Because  
638 agroforestry systems like Aquiares or CATIE sites are spatially heterogeneous, they were expected to violate  
639 the assumptions of a single air temperature and logarithmic wind profile within the canopy. However, the  
640 simulated wind profile for the Aquiares *Coffea* AFS site was based upon a measured profile along a path 3 to  
641 25 m high, and was found largely sufficient for the aim and scope of the model.

642 In summary, the overall accuracy of our model's simulated leaf temperatures (RMSE= 1.4 to 1.7°C, CATIE  
643 temporal experiment) is in the same range as or slightly better than those in other studies. For example, Bailey  
644 et al. (2016a) found an RMSE ranging between 1.4 and 1.9°C, Dauzat et al. (2001) found a 4°C  
645 underestimation for highest temperatures, and the SHAW model (Flerchinger et al., 2015) obtained RMSEs  
646 ranging from 2.8 °C to 4.8 °C.

647 Therefore, MAESPA can provide reasonable simulations of the main processes that determine leaf  
648 temperatures under very large ranges of shading conditions. This capability is a clear advantage of 3D  
649 representations of trees (Pretzsch et al., 2015).

## 650 **Conclusions**

651 Few models of stands and individual trees can provide reasonably accurate, computationally-efficient  
652 simulations of key processes, balances, fluxes, and trends (e.g., latent- and sensible-heat; soil and leaf  
653 temperature; within-canopy air temperature and vapour pressure; thermal, NIR, and PAR radiation; rainwater  
654 throughfall; canopy and soil evaporation; transpiration, infiltration, runoff, and drainage; and carbon transport  
655 via photosynthesis and respiration) altogether (Simioni et al., 2016;Flerchinger et al., 2015). The ability of this  
656 new version of MAESPA to simulate complex stands with a good balance of speed and accuracy positions it  
657 between simple, multi-layer methods and complex ray-tracing models. That balance accrues primarily from  
658 (a) the model's computation of 3D light interception from a simple representation of the trees architecture  
659 through array-grid representation of voxels; and (b) a fast scheme for calculating balances of energy, water,  
660 and carbon. The purpose of this new iterative scheme in MAESPA was to improve the model accuracy by  
661 simulating leaf evaporation at the voxel scale, and by also simulating the within-canopy air temperature and  
662 vapour pressure, thereby obtaining coupled energy and water balances that could be closed iteratively through  
663 convergence of calculated leaf, soil, and canopy air temperatures.

664 The model simulates accurately both simple *Eucalyptus* and complex *Coffea* AFS stands, and is fast enough to  
665 generate yearly plot-scale simulations for partitioning of energy and evapotranspiration. Hence, the model is  
666 sufficiently general to be applicable to diverse species and spatial arrangements, making it a good candidate  
667 for optimisation of (agro-)forestry management. For example, the model can be used to assess the  
668 managements with the best partitioning between soil and leaf evaporation versus plant transpiration, according  
669 to the precipitation regime. MAESPA is also well suited to predicting ecosystem responses to climate  
670 changes, thanks to its process-based functioning.

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691

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- 850
- 851

## 2.4. Conclusion du chapitre

Peu de modèles peuvent simuler avec précision et rapidité les processus clés qui influent sur les bilans d'énergie et d'eau des systèmes forestiers à l'échelle de l'arbre et du peuplement, les flux de chaleur latente et sensible, la température du sol, de l'air et des feuilles, ou encore la transpiration ou l'évaporation. Cependant, MAESPA s'est avéré capable de simuler des systèmes simples et complexes avec un bon équilibre entre rapidité et finesse de description des processus, ce qui le place dans une niche bien particulière entre les modèles multicouches et les modèles complexes comme les modèles à tracé de rayons (ray-tracing models en anglais). Cet équilibre provient principalement (a) du calcul tridimensionnel de l'interception de la lumière à partir d'une représentation simple de l'architecture des arbres (voxels) ; et (b) une méthode rapide pour calculer les bilans d'énergie, d'eau et de carbone. Le but de ce nouveau calcul itératif dans MAESPA était d'améliorer la fidélité du modèle quant aux processus en jeu, en simulant l'évaporation des feuilles à l'échelle du voxel et en simulant la température de l'air et la pression de vapeur à l'intérieur de la canopée. Cette méthode permet de coupler les bilans d'énergie et d'eau, qui sont donc calculés par itération jusqu'à la convergence des températures des feuilles, du sol et de l'air à l'intérieur de la canopée.

Ce modèle est capable de simuler avec justesse des peuplements simples (Eucalyptus) ou complexes (AFS de caféiers), et est suffisamment rapide pour générer des simulations annuelles à l'échelle de la parcelle. Par conséquent, MAESPA est suffisamment générique pour être applicable à diverses espèces et à différentes gestions, ce qui en fait un bon candidat pour l'optimisation de la gestion (agro-) forestière. Par exemple, le modèle peut être utilisé pour évaluer les gestions avec la meilleure répartition entre l'évaporation du sol et des feuilles par rapport à la transpiration des plantes, selon le régime des précipitations. MAESPA est également bien adapté à la prédiction des réponses des écosystèmes aux changements climatiques, grâce à son fonctionnement basé sur les processus.

Finalement, les résultats de ce chapitre ont donc montré que MAESPA est capable de simuler raisonnablement des systèmes de complexité différentes, avec des gestions et des climats variés, pour de nombreux processus tant à l'échelle de l'individu que de la parcelle.





# **Chapitre 3. Modelling yield, net primary productivity, energy, and water partitioning in heterogeneous agroforestry systems: a new coffee agroforestry dynamic model driven by metamodels from MAESPA**

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### 3.1. Introduction au chapitre

Ce chapitre décrit en détail le modèle dynamique de culture de caféier, la démarche de création et d'inclusion des métamodèles de MAESPA, ainsi que le paramétrage du modèle, puis son test sur le site d'Aquières pour le confronter à des données mesurées. Le développement du modèle dynamique s'est fait en s'inspirant de deux autres modèles. D'une part le modèle de Rodríguez et al. (2011) qui permet de reproduire le développement reproductif du caféier qui s'étale sur deux années, et qui peut avoir un comportement de floraison synchrone ou asynchrone selon les conditions phénologiques et environnementales ; et d'autre part le modèle de Van Oijen et al. (2010b) qui simule les caféiers à l'échelle de la parcelle, et qui permet de simuler en partie l'influence de la gestion et du climat. Il a donc été développé dans le but de simuler les bilans d'énergie, d'eau et de carbone de la parcelle, ainsi que la croissance des caféiers et la production de grains de café selon le climat et la gestion. De plus, ce chapitre s'inscrit directement dans la continuité du chapitre précédent car le calcul des variables influencées par la structure de la canopée et le climat à l'échelle de l'individu se fait grâce à l'utilisation de métamodèles de MAESPA, qui a donc été paramétré et validé sur le même site agroforestier d'Aquières.

### 3.2. Résumé en français

Les cycles du carbone et de l'eau, la croissance et les rendements des systèmes agroforestiers du café sont difficiles à modéliser en raison de leur phénologie complexe et du grand nombre de compositions possibles d'espèces d'arbres d'ombrage et de gestions. De plus, l'hétérogénéité spatiale induite par les arbres d'ombrages rend la distribution lumineuse hétérogène, ce qui influence les conditions micro-météorologiques. Peu de modèles ont déjà été utilisés sur ces systèmes, mais aucun d'eux ne représente entièrement l'hétérogénéité spatiale de la canopée tout en étant assez rapide pour prédire l'allocation de carbone des différentes gestions. Pour remédier à ces problèmes, un nouveau modèle dynamique de culture basé sur des processus a été développé pour calculer la NPP, l'allocation du carbone, la croissance, le rendement, et les bilans d'énergie et d'eau des plantations de café selon la gestion, tout en tenant compte des effets de l'hétérogénéité spatiale grâce à l'utilisation de métamodèles issus du modèle 3D MAESPA. Le modèle utilise également des cohortes de bourgeons et de fruits qui permettent d'étaler la distribution de la demande en carbone des fruits tout au long de l'année, pour mieux représenter le développement de la reproduction du caféier.

Le modèle simule correctement la production nette de carbone et son allocation aux différents organes, ainsi que les rendements comparativement aux mesures effectuées lors d'études antérieures sur le même site. De plus, les bilans hydriques et d'énergie sont aussi simulés de manière satisfaisante lorsqu'ils sont comparés à plusieurs années de mesures provenant d'une base de données. Notre méthodologie peut être considérée comme un moyen rapide et flexible d'intégrer des processus qui fonctionnent à plus petite échelle que le fonctionnement intrinsèque d'un modèle cible, nous permettant de développer rapidement des modèles plus complets et plus rapides.





1 3.3. Article scientifique

2 **Modeling Yield, Net Primary Productivity, Energy, And Water**  
3 **Partitioning in Heterogeneous Agroforestry Systems: A New**  
4 **Coffee Agroforestry Dynamic Model Driven by Metamodels From**  
5 **MAESPA**

6 Rémi Vezy<sup>a,b,c\*</sup>, Gueric le Maire<sup>a,b,d</sup>, Mathias Christina<sup>a,b,e</sup>, Selena Georgiou<sup>f</sup>, Pablo Imbach<sup>f</sup>, Hugo G.  
7 Hidalgo<sup>g,h</sup>, Eric J. Alfaro<sup>g,h</sup>, Céline Blitz-Frayret<sup>a,b</sup>, Jean-Paul Laclau<sup>a,b,k</sup>, Delphine Picart<sup>c</sup>, Denis Loustau<sup>c</sup>,  
8 Fabien Charbonnier<sup>a,b,j</sup>, Remko Duursma<sup>i</sup>, Belinda Medlyn<sup>i</sup>, Peter Lehner<sup>l</sup>, Olivier Roupsard<sup>a,b,f</sup>

9 <sup>a</sup>CIRAD, UMR Eco&Sols, F-34398 Montpellier, France.

10 <sup>b</sup>Eco&Sols, Univ Montpellier, CIRAD, INRA, IRD, Montpellier SupAgro, Montpellier, France

11 <sup>c</sup>INRA, UMR 1391 ISPA, F-33140 Villenave d'Ornon, France

12 <sup>d</sup>UNICAMP, NIPE, Campinas, Brazil

13 <sup>e</sup>CIRAD, UR 115, AIDA, 34398 Montpellier, France

14 <sup>f</sup>CATIE, Centro Agronómico Tropical de Investigación y Enseñanza, Turrialba 30501, Costa Rica

15 <sup>g</sup>Escuela de Física, University of Costa Rica, 2060-Ciudad Universitaria Rodrigo Facio San Pedro, San José, CR.

16 <sup>h</sup>Center for Geophysical Research, University of Costa Rica, 2060-Ciudad Universitaria Rodrigo Facio San Pedro.

17 <sup>i</sup>Hawkesbury Institute for the Environment, Western Sydney University, Locked Bag 1797, Penrith, Australia

18 <sup>j</sup>El Colegio de la Frontera Sur, CONACyT research fellow, San Cristóbal de las Casas, 29290 Chiapas, México

19 <sup>k</sup>Universidade de São Paulo, SP, Brazil

20 <sup>l</sup>Cafetalera Aquiares S.A., PO Box 362-7150, Turrialba, 7150, Costa Rica

21 \*Corresponding author. Email address: remi.vezy@cirad.fr (R. Vezy).

22

23 **Abstract**

24 Carbon and water cycles, growth and yields of coffee agroforestry systems are difficult to model because of  
25 their complex reproductive phenology, and of the multitude possible shade tree species and management that  
26 influence the micrometeorological conditions and make the light distribution heterogeneous. Few models have  
27 already been used on these systems, but neither of them account for the 3D effect of shade while being fast  
28 enough to predict carbon allocation along with management effect. To overcome these issues, a new dynamic  
29 process-based growth and yield model was developed to compute plot-scale NPP, carbon allocation, growth,  
30 yield, energy, and water balance of coffee plantations according to management, while accounting for spatial  
31 effects using metamodels from the 3D process-based MAESPA. The model also uses coffee bud and fruit  
32 cohorts for reproductive development to better represent fruit carbon demand distribution along the year.  
33 The model gave satisfactorily results on NPP and carbon mass for all different organs or even yield when  
34 compared to measurements from previous studies on the same site, and when compared to several years of  
35 energy and water balance measurements from a comprehensive database. Our methodology can be thought as  
36 a flexible way to create models that account for processes that work at finer scale, while developing rapidly  
37 more inclusive and faster models.

38 **Keywords:** dynamic crop model; process-based model; MAESPA; metamodel; yield; net primary  
39 productivity; water balance; agroforestry; *Coffea arabica*.

## 40 1. Introduction

41 The key role of dynamic crop models is to help understanding and predicting the effects and interactions  
42 between meteorology, soil, management, climate, species facilitation and competition on the crop  
43 development and yield. Crop models can give insights to the main emerging agricultural challenges to sustain  
44 food security, coming from population growth, the need for sustainable agriculture and ecosystem services,  
45 and climate change (Spiertz, 2012). There is an increasing need to address these issues at global scale to  
46 prospect the different solutions available (Makowski et al., 2014), especially for crops exchanged on the  
47 global market such as wheat, maize, soybean, coffee, or cacao.

48 The ease of development of crop models depends principally on the complexity of the processes at stake on  
49 the system, and on the available data for calibration and validation. Perennial plantations are more complex to  
50 study because their relatively long growing cycle slow down the data acquisition, and because their canopy  
51 heterogeneity can lead to anisotropy for light and for micro-meteorological conditions, such as temperature,  
52 vapor pressure or wind (Luedeling et al., 2014;Luedeling et al., 2016). The paramount complex perennial  
53 systems would certainly be agroforestry system (AFS) (Malézieux et al., 2009), because they present the most  
54 heterogeneous canopies in the vertical and/or horizontal directions, which affect all ecosystem fluxes  
55 (Charbonnier et al., 2013;Soma et al., in prep.;Vezy et al., under review). Yet agroforestry systems have the  
56 potential to enhance ecosystem services (Jose, 2009;Lin, 2010;Taugourdeau et al., 2014), carbon sequestration  
57 (Oelbermann et al., 2004;Jose and Bardhan, 2012), or even mitigate climate pressure on crops (Lin, 2007).

58 *Coffee arabica* production is mostly made under agroforestry systems in Costa Rica because it was found to  
59 improve coffee bean quality and to have the ability to expand the cultivation area to sub-optimal environments  
60 (Muschler, 2001). But these systems are difficult to model due to many factors. First, there are many types of  
61 shade management with highly heterogeneous canopies, ranging from free growing, low density shade trees  
62 like *Cordia alliodora* to high density heavily managed low trees such as banana trees or pollarded *Erythrina*  
63 *poeppigiana* trees (van Oijen et al., 2010a). Second, the coffee phenology itself is complex. It has a two-year  
64 cycle for bud-flower-fruit development (Camargo and Camargo, 2001), its flowering is mostly synchronized  
65 on sub-tropical regions but can also be largely asynchronous on equatorial regions, with consequences on the  
66 distribution of the demand for fruits that will impact the next compartments allocation (Cannell, 1985b). It is  
67 often managed at sprout level, pruned every five to six years to maintain high levels of production. It is also  
68 believed that the reserve compartment may play a large role in bean production, with a biennial dynamic  
69 occurring at resprout level (Cannell, 1985b). Finally, many yield data sets are available at the plot or at the  
70 farm scale, but there are very few comprehensive data sets to calibrate and validate multi-objective models  
71 (e.g. energy, carbon, and water balance, aboveground and belowground biomass, NPP, berry yield...).

72 Important environmental factors to model coffee production are mainly (1) absorbed light and (2) light use  
73 efficiency (LUE) and (3) within canopy temperature to account for shade tree impact on coffee micro-  
74 meteorology to better compute its vegetative growth, maintenance respiration, flower development, and  
75 canopy transpiration. Important biotic factors to model coffee production are (1) shade tree and coffee leaf

76 phenology to adjust light intake, canopy temperature and transpiration, (2) carbon partitioning to compute net  
77 primary productivity (NPP) and then dry mass of each organ and reserves, (3) reproductive organs phenology  
78 from buds, flowers until different fruits stages up to maturation and overripe.

79 Several models are already available for coffee production simulation in full sun or agroforestry. Rodríguez et  
80 al. (2011) proposed a plant dynamic model to simulate coffee in monoculture at branch-scale. It was  
81 calibrated from planting to five years-old (*i.e.* one cycle of production). The strength of this model lies in the  
82 fine phenology and physiological processes of the modelled coffee plant for instance using branch-level  
83 cohorts of flowers and fruits, while flowering is a consequence of microclimate occurring during the previous  
84 year. It also has a pest module for coffee berry borer. The model was successfully calibrated on Colombian  
85 and Brazilian sites, two regions of contrasting climate and flower phenology (subtropical and equatorial). It  
86 has some limitations though. It works at the plot scale, light absorption is computed using the Beer-Lambert  
87 law with a constant coefficient of extinction, and a constant light use efficiency. Furthermore, coffee pruning,  
88 shade trees, water and energy balance and canopy temperature are missing from the model. A second model is  
89 the one from Van Oijen et al. (2010b), which is a plot-scale dynamic coffee agroforestry model. It computes  
90 various types of shade tree management and species, different ecosystem services, is fast because every  
91 subplot of shaded or non-shaded plots are made independent, and can be run under changing climates. The  
92 main limitations of this model would be its light transmission module, which is not considered as a continuum  
93 under shade trees as described in Charbonnier et al. (2013), the lack of any reserve compartment although  
94 being a fruit crop model, LUE is not influenced by the shade management whereas it was found variable in  
95 Charbonnier et al. (2017), and the lack of energy balance and canopy temperature. Two other models were  
96 also applied to coffee agroforestry using 3D light interception modules, first in Dautzat et al. (2001), and then  
97 using the MAESPA model (Charbonnier et al., 2013; Charbonnier et al., 2017; Vezy et al., under review).  
98 Although these models help to compute a precise light intake or plant to plot-scale energy, water and carbon  
99 balance for any shade type, species, management, and climate, their precise state-of-the-art process-based  
100 functioning causes high computation time, and make them unsuitable for long term simulations along full  
101 rotations.

102 Given the high complexity and heterogeneity of agroforestry systems, and their anisotropy (Charbonnier et al.,  
103 2013), it is not considered the best option to use an overly simplified representation of the agroforestry  
104 system. Since MAESPA has recently been demonstrated to give accurate predictions for light distribution,  
105 canopy temperature and water and energy balance in such systems (Charbonnier et al., 2013; Charbonnier et  
106 al., 2017; Vezy et al., under review), it can be used to build surrogate models for any spatial-dependent  
107 variable, to integrate them to a simpler dynamic crop model. These surrogate models are called metamodels,  
108 and were already used in other agronomic or ecological studies for model reduction (Christina et al.,  
109 2016; Marie et al., 2014). Metamodels are simple and instantaneous equations that efficiently compute a given  
110 output of a complex model from the same inputs. In other words, it is a reduction of a complex model that is  
111 meant to emulate the behavior of complex interactions between variables (e.g. spatial heterogeneity) into one

112 short equation. Metamodels can be used to better understand the processes at stake within a model and assess  
113 its sensitivity and uncertainty (Faivre et al., 2013;Christina et al., 2016), for optimization purposes (Razavi et  
114 al., 2012), or to simply make faster and reasonably accurate predictions for a given variable usually computed  
115 by a time-consuming model, with minimum possible error (Marie et al., 2014). It is often used as a solution  
116 for coupling models of different time and/or spatial scales in efficient and easy way, *i.e.* without having the  
117 necessity to iteratively run the finer-scale model, but only run a surrogate computationally efficient model. In  
118 this study, we used MAESPA to calibrate metamodels to simulate any 3D-dependent variable such as diffuse  
119 and direct light extinction coefficient, light use efficiency, transpiration, and leaf temperature (Vezy et al.,  
120 under review). These metamodels are then integrated into a dynamic crop model, to allow this model to  
121 account for spatial heterogeneity while working at plot-scale, with fast development and computation.  
122 Ideally, the best model would combine advantages of models using different processes complexity: the 3D  
123 computation of light, water, energy and carbon of MAESPA, the branch-scale phenology model from  
124 Rodríguez et al. (2011), and then the flexibility for different management, shade tree species and density from  
125 the model of Van Oijen et al. (2010b), while solving all limitations from one to another. Consequently, we  
126 built a dynamic crop model using metamodels from MAESPA for spatial-dependent variables, a plant-scale  
127 phenology inspired from Rodríguez et al. (2011), and the ability to adapt coffee and shade tree management,  
128 density and tree species from Van Oijen et al. (2010b).

129 Therefore, the aims of this paper are:

- 130 (i) To develop metamodels for spatially-dependent variables based on MAESPA, which was already  
131 calibrated and validated for its different modules in coffee agroforestry systems.
- 132 (ii) To make a new coffee agroforestry plot-scale dynamic crop model, using the best features of two  
133 coffee models from the literature and completing with metamodels from MAESPA.
- 134 (iii) To test the new model using qualitative data from literature from other experimental sites along  
135 with literature on the same site and extensive dataset of energy and water balance, yield and  
136 harvest maturity obtained from a long-term observatory.

## 137 **2. Materials and methods**

### 138 **2.1. MAESPA model and metamodel conception**

#### 139 **2.1.1. MAESPA description**

140 MAESPA is a 3D explicit process-based model (Duursma and Medlyn, 2012) used to simulate individual-  
141 scale forest energy, water, and carbon fluxes. This model was already calibrated, used and validated on the  
142 same agroforestry system for its light interception module (Charbonnier et al., 2013), canopy temperature, and  
143 water and energy balance (Vezy et al., under review). MAESPA is particularly suited to simulate agroforestry  
144 system fluxes because it describes the forest at voxel scale, which is a homogeneous representation of a sub-

145 part of the tree crown, and can manage several tree species with their own physiological, physical, and  
146 structural parameters. Thus, MAESPA compute a fine estimation of the light interception, energy, water, and  
147 carbon fluxes for each individual in the forest and for the soil, while considering the canopy spatial  
148 heterogeneity. However, MAESPA doesn't have any carbon allocation or growth process included, and  
149 requires computationally-intensive simulations on thousands of coffee individuals to integrate the shade tree  
150 layer heterogeneity.

### 151 **2.1.2. Metamodels**

152 The purpose of using metamodels in this study was to make a two-layer dynamic crop model able to consider  
153 the 3D canopy heterogeneity effect on fundamental processes, as if it was with a MAESPA-growth model  
154 coupling. Firstly, the main process impacted by canopy complexity is the simulation of light absorbed by the  
155 plants (Charbonnier et al., 2013). Indeed, in dynamic crop models, the absorbed photosynthetically active  
156 radiation (APAR) by the canopy is often computed using the simple Beer-Lambert's law or a derivative, with  
157 a variable leaf area index in time, but a constant extinction coefficient (Van Oijen et al., 2010b). However,  
158 heterogeneous canopies such as the shade trees in AFS coffee plantations tends to violate the assumption of a  
159 constant value for the diffuse ( $K_{Diffuse}$ ) and direct ( $K_{Direct}$ ) light extinction coefficient because the spatial  
160 distribution of the leaf area is not uniform (high gap fraction) and because the leaf area density can change  
161 with time through foliage aggregation (Sampson and Smith, 1993; Sinoquet et al., 2007). Secondly, a  
162 comparison between coffee planted in monoculture and under agroforestry system showed that canopy  
163 complexity affected canopy temperature, water, and energy partitioning (Vezy et al., under review), and  
164 probably photosynthesis because it is related to light interception and transpiration through stomatal  
165 conductance. Therefore, we derived metamodels from MAESPA for the diffuse ( $K_{Diffuse}$ ) and direct  
166 ( $K_{Direct}$ ) shade tree light extinction coefficients, the light use efficiency ( $LUE, g_C MJ$ ), the coffee canopy  
167 temperature ( $T_{canopy}, ^\circ C$ ) and leaf water potential ( $\Psi_{leaf}, MPa$ ), the transpiration ( $Tr, mm day^{-1}$ ) and plant  
168 sensible heat flux ( $H, MJ m^{-2} day^{-1}$ ). The coffee layer was considered homogeneous enough to compute  
169 constant extinction coefficients derived from the MAESPA simulation, and the partitioning parameter  
170 between soil sensible and latent flux was also adjusted using MAESPA outputs.

171 Constructing metamodels from numerous available variables can lead to overfitting due notably to  
172 collinearity, especially when the metamodel is used on previously unknown conditions. This is particularly of  
173 concern in this study, where metamodels come from a one-year simulation of MAESPA only. To overcome  
174 this difficulty, metamodels were built using linear regression, and models were chosen while keeping in mind  
175 a trade-off between the number of explanatory variables (*i.e.* less is better), their nature (*i.e.* genericity and  
176 range of application), their transformation (polynomial, square root...), and its accuracy. Metamodels were  
177 trained on 80% of MAESPA simulation data and checked on 20% remaining validation data to compute out-  
178 of-sample statistics. The input variables of MAESPA that could have been used as predictors for metamodels

179 were either climatic or structural (average plot). Climatic variables included air temperature, vapor pressure,  
 180 PAR, fraction of the diffuse or direct light, wind, or air pressure. Input structural variables were average plot  
 181 leaf area ( $m_{leaves}^2 tree^{-1}$ ), crown height ( $m$ ), trunk height ( $m$ ), crown radius ( $m$ ), trunk diameter ( $m$ ) and all  
 182 derivatives such as leaf area index (LAI,  $m_{leaves}^2 m_{soil}^{-2}$ ), leaf area density (LAD,  $m_{leaves}^2 m_{crown}^{-3}$ ), tree  
 183 density ( $trees ha^{-1}$ ) or crown projection ( $m_{crown}^2 m_{soil}^2$ ).

## 184 2.2. Dynamic crop model description

### 185 2.2.1. Introductory description

186 The model presented in this study is a two vegetation (shade tree and coffee) and soil layer plot scale dynamic  
 187 mechanistic crop model (Murthy, 2004) which aims at simulating coffee plantations growth and yield under  
 188 any shade management while taking account for spatial heterogeneity effects (e.g. light interception, leaf  
 189 temperature, transpiration...). Every layer is assumed to be horizontally homogeneous, and simulated  
 190 sequentially at daily time step. Light absorption, LUE, transpiration, and plant sensible heat flux are all  
 191 considered through metamodels of MAESPA. Coffee can be either planted in monoculture or under  
 192 agroforestry systems of any number of shade tree species layers (e.g. free growing mixed with pollarded tree  
 193 species). The shade tree species share a common allocation model, but have their own parameters, equations  
 194 for metamodels and allometries in their separate module. Currently, light acquisition is the only competition  
 195 between plant layers in the model, whereas all share the same soil water without any retroaction, as observed  
 196 in the considered region (Vezy et al., under review). The model is coded in R language (R Core Team, 2016).

### 197 2.2.2. Light interception and photosynthesis

198 The diffuse ( $APAR_{Diffuse}$ ,  $MJ m^{-2} day^{-1}$ ) and direct ( $APAR_{Direct}$ ,  $MJ m^{-2} day^{-1}$ ) absorbed  
 199 photosynthetically active radiation of each layer are computed using the Beer-Lambert's law of light extinction:

$$APAR_{Diffuse,l,i} = PAR_{AboveDiffuse,i,l} \cdot (1 - e^{-K_{Diffuse,l,i} \cdot LAI_{l,i}}) \quad (1)$$

$$APAR_{Direct,l,i} = PAR_{AboveDirect,i,l} \cdot (1 - e^{-K_{Direct,l,i} \cdot LAI_{l,i}}) \quad (2)$$

200 with  $i$  the day,  $l$  the vegetation layer of consideration,  $PAR_{AboveDiffuse|Direct}$  the diffuse and direct  
 201 photosynthetically active radiation ( $MJ m^{-2} day^{-1}$ ) reaching the layer,  $K_{Diffuse|Direct}$  the light extinction  
 202 coefficient of the layer and  $LAI$  the leaf area index ( $m_{leaf}^2 m_{soil}^{-2}$ ) of the layer.  $PAR_{Above}$  is computed as the  
 203 incoming  $PAR$  minus the  $PAR$  absorbed by upper layer(s) if any. The stand-scale light extinction coefficients  
 204 of the shade tree layer are computed for each day using metamodels from MAESPA, while the extinction  
 205 coefficients of coffee do not vary as much with time, and is therefore taken as constant.



206 The Gross Primary Production ( $GPP, g_C m^{-2} day^{-1}$ ) of each layer is then computed from their respective  
 207 sum of diffuse and direct APAR and light use efficiency ( $LUE, g_C MJ$ ), which is also computed using a  
 208 MAESPA metamodel:

$$GPP_{l,i} = (APAR_{Diffuse,l,i} + APAR_{Direct,l,i}) \cdot LUE_{l,i} \quad (3)$$

### 209 **2.2.3. Maintenance Respiration**

210 Before any partitioning between organs, the available carbohydrate carbon pool ( $Offer, g_C m^{-2} day^{-1}$ ) is  
 211 first supplied to the maintenance respiration requirement, which is computed as the sum of all organs  
 212 maintenance respiration. The maintenance respiration of each organ is computed using its previous day's  
 213 carbon mass ( $CM_{organ}, g_C m^{-2}$ ), following a  $Q_{10}$  formalism as in Dufrêne et al. (2005) :

$$Rm_{organ,l,i} = p_{alive,organ,l} \cdot CM_{organ,l,i-1} \cdot N_{organ,l} \cdot MRN_l \cdot Q_{10,organ,l}^{\frac{T_{organ,l,i} - T_{MR,organ,l}}{10}} \quad (4)$$

214 with  $p_{alive,organ}$  (0-1) the living fraction of the organ,  $CM_{organ}$  ( $g_C m^{-2}$ ) the carbon mass of the organ,  
 215  $N_{organ}$  ( $g_N g_C^{-1}$ ) the nitrogen mass per alive carbon mass unit, and  $MRN$  ( $g_C g_N^{-1} day^{-1}$ ) the respiration rate  
 216 per nitrogen unit,  $Q_{10,organ}$  (1) the temperature response of the respiration,  $T_{organ}$  ( $^{\circ}C$ ) the temperature of the  
 217 organ and  $T_{MR}$  ( $^{\circ}C$ ) the base temperature of maintenance respiration.  $T_{organ}$  being unknown, the air  
 218 temperature is used as a proxy for the shade tree species. For the coffee layer, the temperature is computed  
 219 from a MAESPA metamodel (see below).

### 220 **2.2.4. Carbon offer**

221 A whole plant carbon offer pool is computed from daily GPP, available reserves, and reduced by the plant  
 222 maintenance respiration:

$$Offer_{l,i} = GPP_{l,i} + kres_l \cdot CM_{RE,l,i-1} - Rm_{tot,l,i} \quad (5)$$

223 The reserves available as offer for the day  $i$  are computed as a fraction ( $kres_l$ ) of the carbon mass of the  
 224 reserves ( $CM_{RE,l,i-1}$ ) from the previous day. This method ensures that a fraction of carbon from the reserves  
 225 can be re-allocated the next day, even to the compartments with no demand limit.

### 226 **2.2.5. Carbon allocation to organs**

227 The  $Offer$  is distributed through the different organs using a hierarchical allocation scheme (Lacointe, 2000).  
 228 The priority was assumed to be the wood from shoot+coarse roots first, then fruits, then leaves and fine roots:  
 229 indeed, Charbonnier et al. (2017) reported that shoot allocations remained quite steady whatever the fruit  
 230 biennialty, and we considered here that shoots, and by extension coarse roots, were served first. On the  
 231 contrary, allocation to leaves was the complement of allocation to fruits (low allocation to leaves during years  
 232 of high fruit load) and we assumed that fruits were served just after shoots, the remainder being for leaves and

233 fine roots. The variable fruit allocation can soak up all remaining carbon if the demand is high, then leaf and  
 234 fine roots that can take all the remaining carbon if their demand is high. If their demands are low, it may  
 235 remain some carbon that therefore is stored in the reserves.

236 The *Offer* is first partitioned between Carbon Allocation for shoot wood ( $CA_{shoot}$ ), and stump and coarse  
 237 roots wood ( $CA_{stump+coarse\ roots}$ ) using a constant coefficient ( $\lambda_{organ}$ ) representing a fraction of the offer.

$$CA_{shoot,l,i} = \lambda_{shoot} \cdot Offer_{l,i} \quad (6)$$

$$CA_{stump+coarse\ roots,l,i} = \lambda_{stump+coarse\ roots} \cdot Offer_{l,i} \quad (7)$$

$$\lambda_{shoot} + \lambda_{stump+coarse\ roots} < 1$$

238 The carbon allocation to the coffee fruit is computed as the minimum between the total fruit demand (see  
 239 2.2.10) and the remaining carbon offer pool if any. Fruits are not considered for the shade tree layer.

$$CA_{fruit,i} = \min\left(\sum DE_{Fruit,i}, Offer_{l,i} - CA_{shoots,l,i} - CA_{stump,l,i} - CA_{coarse\ roots,l,i}\right) \quad (8)$$

240 The remaining carbon offer, if any, is then allocated to leaves and fine roots as the minimum between their  
 241 respective offer or demand. Their demand is defined by a parameter, while their offer is computed according  
 242 to a coefficient of allocation ( $\lambda_{remain,organ}$ ) of the remaining carbon (if any):

$$Offer_{leave,l,i} = \max(0, \lambda_{leaves} \cdot (Offer_{l,i} - CA_{shoots,l,i} - CA_{stump+coarse\ roots,l,i} - CA_{fruit,l,i})) \quad (9)$$

$$Offer_{fine\ roots,l,i} = \max(0, \lambda_{fine\ roots} \cdot (Offer_{l,i} - CA_{shoots,l,i} - CA_{stump+coar.roots,l,i} - CA_{fruit,l,i})) \quad (10)$$

$$\lambda_{leaves} + \lambda_{fine\ roots} = 1 \quad (11)$$

$$CA_{leaves,l,i} = \min(DE_{leaves,l,i}, Offer_{leave,l,i}) \quad (12)$$

$$CA_{fine\ roots,l,i} = \min(DE_{fine\ roots,l,i}, Offer_{fine\ roots,l,i}) \quad (13)$$

243 Note that in the above-mentioned equations, the allocation coefficients  $\lambda$  are either applied to the total carbon  
 244 offer, or to the remaining carbon offer, and therefore they do not sum up to one.

245 Finally, if there is any carbon left, it is allocated to the reserves:

$$CA_{reserves,l,i} = \max(0, Offer_{l,i} - CA_{shoots,l,i} - CA_{stump+c\ roots,l,i} - CA_{fruit,l,i} - CA_{leaves,l,i} - CA_{fine\ roots,l,i}) \quad (14)$$

## 246 2.2.6. Net primary production

247 The maintenance respiration is already accounted for before any Carbon allocation (see 2.2.3), but the energy  
 248 used for building new organs creates a loss of carbon in growth respiration. Therefore, the net primary  
 249 production of each organ ( $NPP_{organ}, g_C m^{-2} day^{-1}$ ) is computed using a construction cost coefficient  
 250 ( $\varepsilon_{organ}, g_C g_C^{-1}$ ) on allocated carbon:

$$NPP_{organ,l,i} = \varepsilon_{organ} \cdot CA_{organ,l,i} \quad (15)$$

$$Rg_{organ,l,i} = (1 - \varepsilon_{organ}) \cdot CA_{organ,l,i} \quad (16)$$

$$organ = \{shoot; stump + coarse\ roots; fruits; leaves; fine\ roots\} \quad (17)$$

251 There is no construction cost for the reserves ( $NPP_{reserves} = CA_{reserves}$ )

252 The net primary production of the plant is the sum of the  $NPP_{organ}$  of the considered layer, and the total net  
 253 primary production is the sum of the  $NPP_{organ}$  of all layers.

### 254 **2.2.7. Mortality**

255 Mortality is the result of one or more of the natural mortality (turnover rate), the pruning, or the diseases.  
 256 Natural mortality is computed using an organ-specific lifespan parameter (inverse of the turnover rate), which  
 257 is a proportion of carbon mass from the previous day:

$$M_{natural,organ,l,i} = \frac{CM_{organ,l,i-1}}{lifespan_{organ}} \quad (18)$$

258 The pruning mortality only affects leaves, fine roots, and shoots (branches for the shade trees). It is computed  
 259 as follows for the leaves and shoots:

$$M_{pruning,leaves,l,i} = Pruning\ Intensity_{leaves} \cdot CM_{leaves,l,i-1} \quad (19)$$

$$M_{pruning,shoots,l,i} = Pruning\ Intensity_{shoots} \cdot CM_{shoots,l,i-1} \quad (20)$$

260 The fine roots pruning mortality is made to be directly linked to the leaves pruning intensity using a constant  
 261 parameter:

$$M_{pruning,fine\ roots,l,i} = M_{pruning,leaf,l,i} \cdot m_{rate,fine\ roots} \quad (21)$$

262 The leaf mortality by disease is implemented for coffee leaves only, using a module to compute the American  
 263 Leaf Spot (ALS), computed following Avelino et al. (2007).

264 The total mortality of each organ  $M_{tot,organ}$  is computed as the sum of all its mortalities (natural, pruning,  
 265 disease).

### 266 **2.2.8. Carbon and dry mass of organs**

267 The carbon mass of a compartment is incremented daily by adding the  $NPP_{organ}$  and removing organ  
 268 mortality:

$$CM_{organ,l,i} = CM_{organ,l,i-1} + NPP_{organ,l,i} - M_{tot,organ,l,i} \quad (22)$$

269 The organ dry mass is obtained using the carbon mass and the carbon content of each organ  
 270 ( $C.content_{organ, g_C\ g_{DM}^{-1}}$ ). For the carbon mass of the reserves ( $CM_{RE}$ ),  $NPP_{organ,l,i}$  is replaced by the  
 271 carbon allocated to the reserves on the day  $i$  and  $M_{tot,organ,l,i}$  is replaced by the Carbon consumption of the  
 272 day  $i$ .

### 273 **2.2.9. Branch nodes**

274 The number of branches vegetative nodes is impacted by the mean air temperature during vegetative growth  
 275 (Drinnan and Menzel, 1995), independently of the shoot dry mass. The number of vegetative nodes is  
 276 computed as:

$$Nodes_i = LAI_i \cdot Ratio_{Nodes\ to\ LAI_{20^\circ C}} \cdot COEF_{Nodes\ year} \quad (23)$$

277 where  $LAI_i$  is the leaf area index of the coffee layer on day  $i$ ,  $Ratio_{Nodes\ to\ LAI_{20^\circ C}}$  is the ratio of the number of  
 278 nodes per  $LAI$  unit at  $20^\circ C$ , and  $COEF_{Nodes\ year}$  is an empirical correction coefficient, which takes into  
 279 account the mean temperature during the vegetative growing period ( $T_{gp}$ ,  $^\circ C$ ) derived from data in Drinnan  
 280 and Menzel (1995):

$$COEF_{Nodes\ year} = 0.42 + 0.26 \cdot T_{gp} - 0.02 \cdot T_{gp}^2 + 0.00055 \cdot T_{gp}^3 \quad (24)$$

### 281 2.2.10. Fruit development

282 Coffee fruit production is a two-year process, therefore the reproductive organ development is computed with  
 283 a different model. The reproduction module is mostly derived from Rodríguez et al. (2011), but upscaled to  
 284 the whole-plant. Two main development processes are computed in the model: the bud cohorts, and then the  
 285 fruit cohorts of the following year. The bud has two stages of development itself, while the fruit has five. Buds  
 286 are initiated during the period  $BIP_{Start}$  to  $BIP_{End}$ . The buds start appearing ( $BIP_{Start}$ ) every day in daily  
 287 cohorts on branches nodes as soon as the cumulative sum of the degree days ( $dd$ ) after the end of the  
 288 vegetative development ( $VG_{end}$ ) reaches the value  $T_{ffb}$  (time of first floral buds) degree days. The number  
 289 of days ( $d_{T_{ffb}}$ ) between  $VG_{end}$  and  $BIP_{Start}$  is then computed as:

$$\left\{ \begin{array}{l} \text{find } d_{T_{ffb}} \text{ when : } \sum_{VG_{end}}^{d_{T_{ffb}}} dd = T_{ffb} \\ BIP_{Start} = VG_{end} + d_{T_{ffb}} \end{array} \right\} \quad (25)$$

290 Once initiated, each bud cohort develop during  $dd_{bud\_stage\_1}$  degree days until entering dormancy (bud stage  
 291 2). The dormancy can potentially be broken once the cumulated rainfall during bud dormancy reaches the  
 292  $P_{break}$  millimetres threshold, which is the minimum amount of rainfall required for dormancy break. If  $P_{break}$   
 293 is not reached within 1722 degree-days after the first dormancy, buds are considered dessicated. The buds stop  
 294 appearing ( $BIP_{End}$ ) the instant when first flowers may potentially appear, *i.e.* when the conditions for the first  
 295 bud cohort to develop until the first flowering is reached. Flowers may appear 100 degree-days after potential  
 296 bud break dormancy.

$$\left\{ \begin{array}{l} \text{Find } d_{Pot.Bud} \text{ when : } \sum_{BIP_{Start}}^{d_{Pot.Bud}} dd = dd_{bud\_stage\_1} \\ \text{Find } d_{Pot.Break} \text{ when : } \sum_{d_{Pot.Bud}}^{d_{Pot.Break}} dd = P_{break} \\ \text{Find } d_{Pot.flower} \text{ when : } \sum_{d_{Pot.Break}}^{d_{flower}} dd = dd_{bud\_stage\_2} \end{array} \right.$$

$$BIP_{End} = BIP_{Start} + d_{Pot.Bud} + d_{Pot.Break} + d_{Pot.flower} \quad (26)$$

298 Where  $dd_{bud\_stage\_1}$ ,  $dd_{bud\_stage\_2}$  and  $P_{break}$  are cumulated degree-days or precipitation threshold values,  
 299 and  $d_{Pot.Bud}$ ,  $d_{Pot.Break}$  and  $d_{flower}$  are the date when these threshold are successively reached (end of first  
 300 bud stage, end of second bud stage with bud dormancy break, and date of bud flowering).

301  
 302 Once the bud initiation period known, the rate of bud initiation in each day between  $BIP_{Start}$  and  $BIP_{End}$   
 303 depends on the incoming radiation and temperature occurring that day, and on the number of nodes to  
 304 supports the buds. This computation is made following Eq.12 from Rodríguez et al. (2011) adapted to the  
 305 whole-plant level instead of branch level. As for the number of nodes, the number of floral buds initiated  
 306 ( $Bud.Init$ ) is impacted by the average diurnal air temperature within the coffee canopy during their growth  
 307 ( $MTcan_{BGP}$ ). This temperature effect is implemented as a correction factor of the number of initiated buds if  
 308  $MTcan_{BGP}$  is higher than  $23^{\circ}C$ , which is derived from Drinnan and Menzel (1995) data:

$$Bud.Init_i = \begin{cases} (a - b \cdot RAD) \cdot Nodes_i \cdot dd & \text{if } MTcan_{BGP} < 23^{\circ}C \\ (a - b \cdot RAD) \cdot Nodes_i \cdot dd \cdot (3.29 - 0.1 * MTair_{BGP}) & \text{if } MTcan_{BGP} \geq 23^{\circ}C \end{cases} \quad (27)$$

309 Each bud initiated on day  $i$  is considered to belong to the bud cohort of this day. There are as many cohorts as  
 310 days between  $BIP_{Start}$  and  $BIP_{End}$ . If all these conditions are met, the buds from the cohort pass onto fruit  
 311 stage 1 (flower) with a proportion  $p_{break}$ , which is related to the leaf water potential ( $\Psi_{leaf}, MPa$ ):

$$p_{break,i} = \frac{1}{1 + e^{a+b \cdot \Psi_{leaf}}} \quad (28)$$

312 Therefore, all buds from the initiated cohort on day  $i$  may or may not progressively reach the fruit stage until  
 313  $dd_{stage_2}$ , depending on the conjunction of three factors: the mean diurnal air temperature within the coffee  
 314 canopy during bud growth, the rainfall regime and amount during bud growth, and the leaf water potential  
 315 ( $\Psi_{leaf}, MPa$ ) of the coffee. These conditions reflects the need of a dry period followed by an intense rainfall  
 316 for best dormancy break (Rodríguez et al., 2011).

317 If the buds effectively break dormancy, they enter the fruit stage by forming a flower (stage 1 fruit). Then, the  
 318 fruits develop from pin, green, yellow (stages 1,2,3) and then become mature (stage 4) until overripe (stage 5),  
 319 where they fall on the ground. Each bud breaking dormancy on day  $i$  from the different bud cohorts forms a  
 320 new cohort of fruits. The fruit cohort will then enter the carbon allocation scheme and then experience the  
 321 successive maturation stages. The cohort carbon demand increases from the day  $i$  until  $d_{ov}$  following a  
 322 logistic distribution (Eq.(29)) that distribute the optimal carbon demand of all fruits from the cohort along  
 323 their growth period (Eq. (30)).  $d_{ov}$  is the day at which the cohort will overripe and fall onto the ground. It is  
 324 found by computing the cumulative number of degree days until  $dd_{ov}$  degree-days, which is the number of  
 325 degree days a cohort take to overripe. The inflexion date of the logistic distribution  $d_{inf}$  is found similarly  
 326 using  $dd_{infl}$ . Thereby, the total fruit carbon demand of any day  $i$  is computed as the sum of the demand of all  
 327 cohorts growing on the coffee this day (Eq. (31)). If the fruits are not harvest before they overripe, they are  
 328 removed from the coffee.

$$DD_{Cohort,i:d_{Ov}} = \frac{1}{1+e^{-k_{scale} \cdot ([i:d_{Ov}] - d_{inf})}} - \frac{1}{1+e^{-k_{scale} \cdot ([i+1:d_{Ov}+1] - d_{inf})}} \quad (29)$$

$$DE_{Cohort,i:d_{Ov}} = NFruits_i * OptDE * DD_{Cohort,i:d_{Ov}} \quad (30)$$

$$DE_{Fruit,i:d_{Ov}} = DE_{Fruit,i:d_{Ov}} + DE_{Cohort,i:d_{Ov}} \quad (31)$$

329 where  $d_{Ov}$  is the day on which the fruit will overripe,  $d_{inf}$  is the day at which fruit is at fifty percent of  
 330 growth,  $DD_{Cohort}$  is the relative distributing function for the cohort's demand along the cohort growing period  
 331 (*i.e.* logistic distribution with a sum of 1),  $DE_{Cohort}$  ( $g_C m^{-2} day^{-1}$ ) is the effective carbon demand of the  
 332 cohort distributed along the period, with  $NFruits_i$  the total number of stage 1 fruits from the cohort on day  $i$   
 333 and  $OptDE$  ( $g_C Fruit^{-1}$ ) is the optimal non-limited carbon demand per fruit.  $DE_{Fruit}$  ( $g_C m^{-2} day^{-1}$ ) is the  
 334 total carbon demand of all cohorts, that is incremented progressively by each cohort demand.

335 The fruit demand could be considered as the optimal fruit growth, without any offer limitations. Hence, it is a  
 336 sink strength that depends on the number of fruits and the degree days, and is independent of the carbon offer  
 337 from photosynthesis and reserves. The allocation of carbon to fruits is constrained either by fruit demand or  
 338 carbon offer (Eq. (8)). The fruit mass is then computed as in Equ. (22) with the mortality being the overripen  
 339 fruits.

340 Coffee bean quality is also computed using the fruit sucrose content of each fruit cohort from the number of  
 341 days after flowering following the model of Pezzopane et al. (2012). The harvest maturity is then computed  
 342 as:

$$Mat_i = \frac{[Sucrose_i]}{[Sucrose_{Opt}]} \cdot 100 \quad (32)$$

343 with  $[Sucrose_i]$  being the sucrose concentration at day  $i$ , and  $[Sucrose_{Opt}]$  the optimal sucrose concentration  
 344 of the coffee bean.

345 Harvest is made once per growing season, on the first day when the total dry mass of the fruits starts to  
 346 decrease due to over maturation. This method ensures the harvest is made at the maximum of production, and  
 347 lead to best yield with high harvest maturity.

### 348 2.2.11. Allometries

349 In addition to the shared allocation scheme, each tree species has its own allometries in its parameter file. Any  
 350 kind of allometries can be implemented, and can then be used for metamodels or to compute informative  
 351 outputs such as stem volume or trunk diameter. For example, in this study, we computed the LAD (Leaf Area  
 352 Density,  $m_{leaves}^2 m_{crown}^{-3}$ ) to use it as a possible input for the light extinction coefficients.

### 353 2.2.12. Soil, water, and energy

354 The soil and water balance module are inspired from the BILJOU model (Granier et al., 2012) which already  
 355 was parameterized for this coffee agroforestry system (Gómez-Delgado et al., 2011). It has 3 layers from 0 to

356 1.25m, 1.25 to 1.75 and 1.75 to 3.75m respectively, thus covering the whole rooting profile of coffee in the  
357 same site (Defrenet et al., 2016). The energy balance is computed using the defaults equations from BILJOU,  
358 except for variables that were found very sensitive to complex canopy structure (Vezy et al., under review),  
359 which were simulated using MAESPA metamodels: shade tree and coffee transpiration and sensible heat,  
360 coffee canopy temperature (used for its maintenance respiration), leaf water potential. The soil evaporation  
361 computation of BILJOU depends on a partitioning parameter between sensible and latent flux, which was  
362 adjusted using MAESPA outputs.

### 363 **2.3. Study sites and measurements**

364 The reference coffee agroforestry system is located near Aquiares in Costa Rica (9°56'19''N, 83°43'46''W,  
365 1040 m.a.s.l) in the 660 ha plantation of the Aquiares farm. It consists in *Coffea arabica* (var. *Caturra*)  
366 planted at a high density of 6300 plants ha<sup>-1</sup> under free growing low density (7.4 trees ha<sup>-1</sup>) *Erythrina*  
367 *poeppigiana* shade trees. The low shade tree density management forms highly spatially heterogeneous plots.  
368 Coffee shoots are selectively pruned approximately every 5 to 6 years to avoid production drop due to  
369 exhaustion. A 1.3 ha research plot located within the farm was monitored since 2009 for water and energy  
370 balance by the CoffeeFlux project (<http://www.umr-ecosols.fr/index.php/en/recherche/projets/53-coffee-flux>).  
371 Data is available in the FLUXNET 2015 dataset (CR-AqC 2009-2016). The mean annual air temperature is  
372 19.5°C and the mean annual rainfall is 3037 mm (from 2009 to 2015), with a dry season of approximately one  
373 month in mars. Shade trees were pollarded twice a year from 1979 until 2000, and then grew freely until the  
374 end of the cycle. Further information on the site can be found in Gómez-Delgado et al. (2011), Charbonnier et  
375 al. (2013) or Taugourdeau et al. (2014).

### 376 **2.4. Model parameterization**

377 MAESPA model was parameterized according to Vezy et al. (under review) and was run on a sub-plot of  
378 4176 coffee sprouts and fourteen shade trees at 30 minutes time-step throughout the year 2011. Metamodels  
379 were then built from daily plot scale aggregations of MAESPA outputs and integrated into the dynamic crop  
380 model. The metamodels were made using linear regression with MAESPA input variables as predictors. The  
381 MAESPA dataset created from the simulations of 2011 was taken as a representative sample of most of the  
382 conditions of the growing cycle, presenting yearly climate variations, a highly variable shade tree LAI due to  
383 total leaf fall, and highly variable coffee structure, with resprouts of different ages from 0 to 5 years old. The  
384 dynamic crop model was run from January 1979 until December 2016 at daily time-step. The input climate for  
385 the dynamic crop model comes from the CoffeeFlux project between 2009 and 2016, and was computed  
386 between 1979 and 2008 using the method and data described in Hidalgo et al. (2016). The values and sources  
387 of the parameters used in the dynamic crop mode lare given in Table 3 for climate and coffee, Table 4 for the  
388 shade tree species, and Table 5 for the soil parameters for the BILJOU module.

389 Table 3. Parameters used in the dynamic crop model.

Parameter	Unit	Value	Description	Source
<i>Climate</i>				
LatitudeCF.deg	degree	9.93833	Latitude	This study
LongitudeCF.deg	degree	-83.728	Longitude	This study
TimezoneCF		6	Time-zone	This study
Elevation_m	m	1040	Elevation	This study
SlopeAzimut_deg	degree	180	Slope direction	This study
Slope_pc	degree	5	Slope	This study
H.Coffee	m	1.2	Coffee height, for zht and zo	This study
H.grass	m	0.12	Understory height (zht and zo)	This study
H.erythrina	m	20	Shade tree height (zht and zo)	This study
H_Meas	m	25	Climate data meas. height	This study
stocking	Plant ha <sup>-1</sup>	6300	Coffee planting density	This study
<i>Coffee light interception</i>				
K <sub>Diffuse</sub>	0-1	0.39	Diffuse light extinction coeff.	This study
K <sub>Direct</sub>	0-1	0.34	Direct light extinction coeff.	This study
<i>Vegetative development</i>				
AgeCofMax	Year	40	Max. length of plantation cycle	This study
AgePruning	Year	5	First pruning age	Meylan (2012)
date_pruning	DOY	74	Day of year of pruning	This study
SLA	m <sup>2</sup> <sub>leaf</sub> kg <sub>DM</sub> <sup>-1</sup>	10.9	Specific leaf area	Charbonnier et al. (2017) <sup>(1)</sup>
DE_Leaves	g <sub>C</sub> m <sup>-2</sup>	0.966	Leaf maximum demand	This study
PrunInt_Leaves		0.26	Fraction of pruned leaf DM	This study
RNL20	Node LAI <sup>-1</sup>	91.2	Ref. n° of nodes per LAI unit at 20°C	Drinnan and Menzel (1995) <sup>(1)</sup>
VG_Start	DOY	105	Beginning of the vegetative growth	Meylan (2012)
VG_End	DOY	244	End of the vegetative growth	Meylan (2012)
kres	0-1	0.329	Max. reserves use per day	This study
λshoot	0-1	0.041	Allocation to resprout wood	This study
λStumpCoarseRoot	0-1	0.02;0.045	Alloc. to perennial wood at age 0/40	This study
λLeaf_remain	0-1	0.94	Remaining carbon alloc. to leaves	This study
λFineRoot_remain	0-1	0.06	Remaining carbon alloc. to fine roots	This study
lifespanLeaf	day	265	Leaf lifespan	Charbonnier et al. (2017)
lifespanRsWood	day	8000	Resprout lifespan	van Oijen et al. (2010a) <sup>(1)</sup>
lifespanStump_C.Root	day	14600	Perennial wood lifespan	This study
lifespanFineRoot	day	365	Fine roots lifespan	Defrenet et al. (2016)
m_fineroots		0.001	fine root to leaf pruning	This study
CContent_Fruit	g <sub>C</sub> g <sub>DM</sub> <sup>-1</sup>	0.4857	Fruit dry mass carbon content	Charbonnier et al. (2017)
CContent_Leaf	g <sub>C</sub> g <sub>DM</sub> <sup>-1</sup>	0.463	Leaf dry mass carbon content	Charbonnier et al. (2017)
CContent_shoot	g <sub>C</sub> g <sub>DM</sub> <sup>-1</sup>	0.463	Resprout wood dry mass C content	Charbonnier et al. (2017)
CContent_Stump_C.Root	g <sub>C</sub> g <sub>DM</sub> <sup>-1</sup>	0.475	Perennial wood dry mass C content	Charbonnier et al. (2017)
εFruit	g <sub>C</sub> g <sub>C</sub> <sup>-1</sup>	0.708	Fruit growth respiration cost	Dufrêne et al. (2005) <sup>(1)</sup>
εLeaf	g <sub>C</sub> g <sub>C</sub> <sup>-1</sup>	0.767	Leaf growth respiration cost	Dufrêne et al. (2005) <sup>(1)</sup>
εFineRoot	g <sub>C</sub> g <sub>C</sub> <sup>-1</sup>	0.781	Fine roots growth respiration cost	Dufrêne et al. (2005) <sup>(1)</sup>
εShoot	g <sub>C</sub> g <sub>C</sub> <sup>-1</sup>	0.833	Shoot wood growth resp. cost	Dufrêne et al. (2005) <sup>(1)</sup>
εStumpCoarseRoot	g <sub>C</sub> g <sub>C</sub> <sup>-1</sup>	0.762	Perennial wood growth resp. cost	Dufrêne et al. (2005) <sup>(1)</sup>
NContentFruit	mg <sub>N</sub> g <sub>C</sub> <sup>-1</sup>	22	Fruit Nitrogen content	van Oijen et al. (2010a)
NContentLeaf	mg <sub>N</sub> g <sub>C</sub> <sup>-1</sup>	6.7	Leaf Nitrogen content	Cambou (2012)
NContentRsWood	mg <sub>N</sub> g <sub>C</sub> <sup>-1</sup>	2.7	Resprout wood Nitrogen content	Cambou (2012)
NContentStump_C.Root	mg <sub>N</sub> g <sub>C</sub> <sup>-1</sup>	1.5	Perennial wood Nitrogen content	Cambou (2012)
NContentFineRoot	mg <sub>N</sub> g <sub>C</sub> <sup>-1</sup>	19.8	Fine roots Nitrogen content	van Praag et al. (1988)
Q10Fruit	1	2.2	Temperature effect on Rm	This study
Q10Leaf	1	2.1		Vose and Bolstad (1999)
Q10RsWood	1	2.8		Damesin et al. (2002)
Q10StumpCoarseRoot	1	1.7		Damesin et al. (2002)
Q10FineRoot	1	2.2		Epron et al. (2001)
MRN	g <sub>C</sub> g <sub>N</sub> <sup>-1</sup> d <sup>-1</sup>	0.1584		Ryan (1991) <sup>(1)</sup>
PaliveFruit;Leaf;Fine root	0-1	1	Percentage of living cells	
PaliveRsWood	0-1	0.37		



390 **Table 2 (continued). Parameters used in the dynamic crop model.**

Parameter	Unit	Value	Description	Source
<i>Reproductive development</i>				
a_Budinit	<i>Buds day</i> <sup>-1</sup>	0.00287	Number of buds initiated per day	Rodríguez et al. (2011)
b_Budinit	1	-4.1. e <sup>-6</sup>		Rodríguez et al. (2011)
Tffb	<i>Degree day</i>	4000	Time of first floral buds	Rodríguez et al. (2011)
a_p	1	5.78	Bud dormancy break probability from	Rodríguez et al. (2011);Drinnan
b_p	1	1.90	leaf water potential	and Menzel (1995)
Rain_BudBreak	<i>mm</i>	10	Cumulative rain to break bud dormancy	Zacharias et al. (2008)
Age_Maturity	<i>Year</i>	3	First age of flowering after planting	van Oijen et al. (2010a)
VFF	<i>Degree day</i>	5500	Very first flowering of Coffee plant	Rodríguez et al., 2001
Bud_stage1	<i>Degree day</i>	840	Bud stage 1	van Oijen et al.
Bud_stage2	<i>Degree day</i>	2562	Bud stage 2	(2010a);Meylan (2012)
<i>dd<sub>mat</sub></i>	<i>Degree day</i>	2836	From pinhead until full maturation (stage	Rodríguez et al. (2011)
<i>dd<sub>ov</sub></i>	<i>Degree day</i>	3304	From pinhead until over-maturation	
kscale	1	0.05	Empirical coefficient for fruit growth	
SF_Ratio	0-1	0.675	Fruit to seed dry mass ratio	Wintgens (2004)
<i>Sucrose accumulation</i>				
S_a	<i>[sucrose]</i>	5.3207		Pezzopane et al. (2012)
S_b	1	-28.556	Parameters to model sucrose	Pezzopane et al. (2012)
S_x0	<i>Degree day</i>	190.972	accumulation into Coffee fruit	This study
S_y0	<i>[sucrose]</i>	3.4980		Pezzopane et al. (2012)
MeanBerriesDM	<i>g<sub>DM</sub></i>	0.246	Optimum berry dry mass	

<sup>(1)</sup>Parameter either tuned starting from source data or adapted from it.

391  
392

393  
394**Table 4. Parameters used in the dynamic crop model for shade Tree (*E.poeppigiana*). The parameter names are as used in the model.**

Parameter	Unit	Value	Description	Source
<i>Vegetative development</i>				
SLA	$m_{Leaf}^2 kg_{DM}$	24.36	Specific leaf area	This study
DE_Leaves	$g_C m^{-2}$	0.966	Leaf maximum demand	This study
$\lambda_{Stem}$	0-1	0.13	Alloc. to stem	This study
$\lambda_{Branch}$	0-1	0.23	Alloc. to branches	This study
$\lambda_{CoarseRoot}$	0-1	0.08	Alloc. to coarse roots	This study
$\lambda_{Leaf}$	0-1	0.3	Alloc. to leaves	This study
$\lambda_{FineRoot}$	0-1	0.26	Alloc. to fine roots	This study
lifespanBranch	day	3650	Branch life span	This study
lifespanLeaf	day	47.71	Leaf life span	This study
lifespanFineRoot	day	81	Fine root life span	This study
lifespanCoarseRoot	day	7300	Coarse root life span	This study
CContent	$g_C g_{DM}^{-1}$	0.42	Mean tree dry mass carbon content	van Oijen et al. (2010a);Nygren et al. (1996)
CContent_leaf	$g_C g_{DM}^{-1}$	0.562	Leaf dry mass carbon content	Oelbermann et al. (2005)
CContent_wood	$g_C g_{DM}^{-1}$	0.438	Wood dry mass carbon content	Oelbermann et al. (2005)
$\varepsilon$	$g_C g_C^{-1}$	0.67	Growth respiration cost	This study
NContentBranch	$g_N g_C^{-1}$	0.0092	Branch Nitrogen content	van Oijen et al. (2010a)
NContentStem	$g_N g_C^{-1}$	0.02	Stem Nitrogen content	van Oijen et al. (2010a)
NContentCoarseRoot	$g_N g_C^{-1}$	0.0092	Coarse root Nitrogen content	van Oijen et al. (2010a)
NContentFineRoot	$g_N g_C^{-1}$	0.0453	Fine root Nitrogen content	van Oijen et al. (2010a)
Q10CoarseRoot	1	2.1	Temperature effect on Rm	This study
Q10Leaf	1	2.1	Temperature effect on Rm	Vose and Bolstad (1999)
Q10Branch	1	2.8	Temperature effect on Rm	Damesin et al. (2002)
Q10Stem	1	1.7	Temperature effect on Rm	Damesin et al. (2002)
Q10FineRoot	1	2.1	Temperature effect on Rm	Epron et al. (2001)
PaliveBranch	0-1	0.33	Percentage of living cells	Dufrêne et al. (2005)
PaliveStem	0-1	1	to Percentage of living cells	This study
PaliveCoarseRoot	0-1	0.21	Percentage of living cells	Dufrêne et al. (2005)
PaliveLeaf, FineRoot	0-1	1	Percentage of living cells	This study
<i>Allometries</i>				
LAD_max	$m_{Leaf}^2 m^{-3}$	0.75	Max leaf area density	Charbonnier et al. (2013) <sup>(1)</sup>
AgePruning	year	1:21	Ages at which trees are pruned	This study
WoodDensity	$kg_{DM} m^{-3}$	250	Wood density	Nygren et al. (1996)
Stocking	tree ha <sup>-1</sup>	7.38	Tree density	Taugourdeau et al. (2014)

<sup>(1)</sup>Parameter either tuned starting from source data or adapted from it.395  
396

397 **Table 5. BILJOU sub-module parameters**

Parameter	Unit	Value	Description	Source
TotalDepth	<i>m</i>	3.75		This study
Wm1	<i>mm</i>	210	Minimum water content, layer 1	This study
Wm2; Wm3	<i>mm</i>	58; 64	Minimum water content, layer 2 and 3	This study
Wf1	<i>mm</i>	290	Field capacity, layer 1	This study
Wf2; Wf3	<i>mm</i>	66; 69	Field capacity, layer 1 and layer 3	This study
IntercSlope	<i>mm LAI<sup>-1</sup></i>	0.2	Rainfall interception	This study
WSurfResMax	<i>mm</i>	120	Max. water on the surface reservoir	This study
fc	<i>mm day<sup>-1</sup></i>	13.4	Min. infiltration capacity	This study
alpha	<i>1</i>	101.561	Coeff. for max. inflit. capacity	This study
kB	<i>day-1</i>	0.038	Discharge coeff. for surface runoff	This study
k_Rn	<i>0-1</i>	0.7	extinction coeff. for Rn to soil	This study
Soil_H_LE_partitioning	<i>%</i>	0.70	Soil energy partitioning coefficient	This study

398 **3. Results**399 **3.1. Metamodels**

400 The metamodels for shade tree  $K_{Diffuse}$  and  $K_{Direct}$  are presented in Table 6, and were computed using the  
401 shade tree LAD ( $LAD_{Tree}, m^2 m^{-3}$ ) only as a predictor. LUE ( $g_C MJ^{-1}$ ) depending more on the environment  
402 than the structure, its metamodel was made using climate inputs. The other metamodels for plant transpiration  
403 ( $Tr, mm$ ), sensible fluxes ( $H, MJ m^{-2}$ ), coffee canopy temperature ( $Tr, mm$ ) and leaf water potential  
404 ( $\Psi_{leaf}, MPa$ ) are also presented in Table 6.

405 The performance of the metamodels is assessed in Figure 19, which shows that despite being simple in  
406 structure, the metamodels are in agreement with the simulations of MAESPA throughout the whole year  
407 simulated (2011). Indeed, all metamodels gave high  $R^2$  and low RMSE, except for  $K_{Direct}$ , which failed to  
408 catch the high day-to-day variability, but still followed the overall trend. Highest errors for all metamodels but  
409  $K$  and  $LUE$  was found around September, where MAESPA  $T_{Canopy}$  iterations didn't converge well. The  
410 variability and the interaction between the predictors are on the same range in this one-year MAESPA  
411 simulation dataset than on the application dataset.

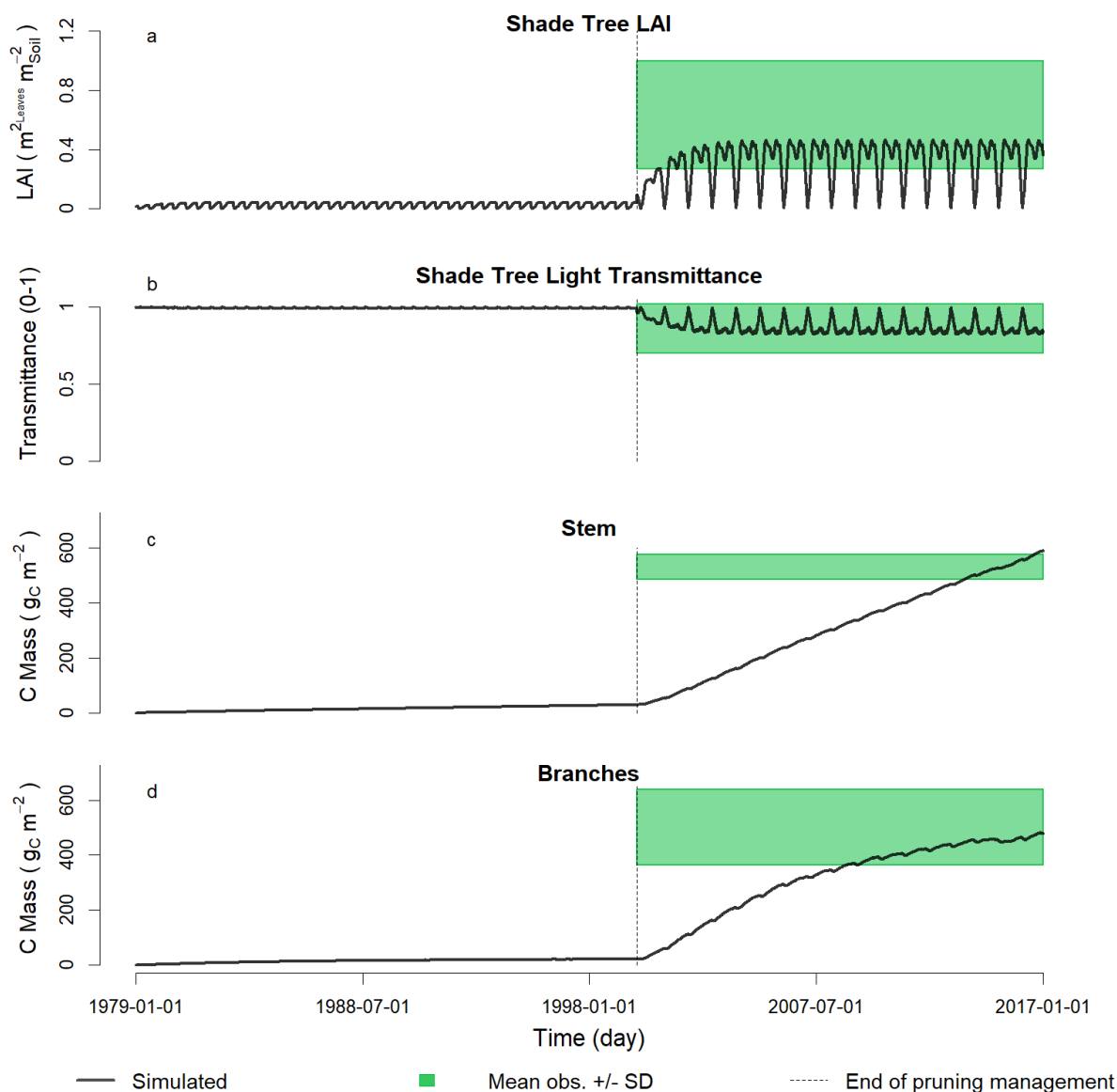
412

413 **Table 6. MAESPA metamodel equations. Where  $T_{air}$  ( $^{\circ}C$ ) and  $VPD_{air}$  ( $hPa$ ) the air temperature and vapor pressure deficit**  
 414 **measured above canopy,  $F_{BEAM}$  (%) the beam fraction of the light and  $PAR_{Above}$  ( $MJ\ m^{-2}\ day^{-1}$ ) the photosynthetically**  
 415 **active radiation reaching the coffee layer (i.e. atm. PAR not absorbed by the shade tree layer),  $\Psi_{soil}$  the soil water potential**  
 416 **( $MPa$ ).**

Metamodel	RMSE	R <sup>2</sup>
$K_{Diffuse,Tree} = 0.6161 - 0.5354 \cdot LAD_{Tree}$	0.02	0.945
$K_{Direct,Tree} = 0.4721 - 0.3973 \cdot LAD_{Tree}$	0.06	0.582
$LUE_{Coffee} = 2.2045 + 0.0116 \cdot T_{air} + 0.00877 \cdot VPD - 1.799 \cdot \sqrt{F_{BEAM}} - 0.2686 \cdot \sqrt{PAR_{Above}}$	0.06	0.977
$LUE_{Tree} = 2.59906 + 0.10707 \cdot T_{air} - 0.02552 \cdot VPD + 3.86372 \cdot F_{BEAM} - 0.34895 \cdot PAR_{Above}$	0.24	0.893
$Tr_{Coffee} = 0.40813 - 0.09301 \cdot T_{air} - 0.11061 \cdot VPD + 2.25512 \cdot F_{BEAM} + 0.79575 \cdot PAR_{Above}$	0.15	0.87
$Tr_{Tree} = 0.021820 \cdot VPD - 0.016112 \cdot T_{air} + 0.942021 \cdot APAR_{Tree} - 1.397349 \cdot F_{BEAM} + 0.004328$ $\cdot LAI_{Tree}$	0.13	0.908
$H_{Coffee} = 0.40813 - 0.09301 \cdot T_{air} - 0.11061 \cdot VPD + 2.25512 \cdot F_{BEAM} + 0.79575 \cdot PAR_{Above}$	0.48	0.956
$H_{Tree} = 0.06241 + 0.75584 \cdot APAR_{Direct,Tree} - 0.82677 \cdot APAR_{Diffuse,Tree} - 0.08356 \cdot LAI_{Tree}$ $- 0.61423 \cdot LE_{Tree}$	0.05	0.905
$T_{canopy,Coffea} = -0.07741 + 0.995 \cdot T_{air} - 0.0695 \cdot VPD - 1.8798 \cdot F_{BEAM} + 0.1962 \cdot PAR_{Above}$	0.43	0.923
$\Psi_{leaf,Coffea} = 0.08053 - 0.01657 \cdot VPD + 0.7227 \cdot F_{BEAM} - 0.04751 \cdot PAR_{Above} + 0.85328 \cdot \Psi_{soil}$	0.03	0.942

### 417 3.2. Growth and yield

418 Shade tree LAI remained very low while under pruning between the start of the planting until year 2000, and  
 419 then grew rapidly to reach a plateau of ca.  $0.6\ m^2\ m^{-2}$  five years after the end of pruning (Figure 18). All  
 420 leaves of *E. poeppigiana* start falling naturally between January and February, and resume growth until May.  
 421 Despite a low density, the shade tree transmits only 86% of the light in average when growing freely, with a  
 422 minimum of 82% when its LAI is at maximum. The simulated dry mass of tree stem and branches represented  
 423 2.3% of the total plot carbon mass before 2000, but grew rapidly until representing 15 and 12% of the total  
 424 carbon mass each at the end of the cycle. Stem mass always increased linearly, but its growth rate was higher  
 425 when not pruned due to the height fold increase in its NPP (Table 7). Branch mass grew slower due to higher  
 426 mortality, which is linked to its carbon mass in the model.



427

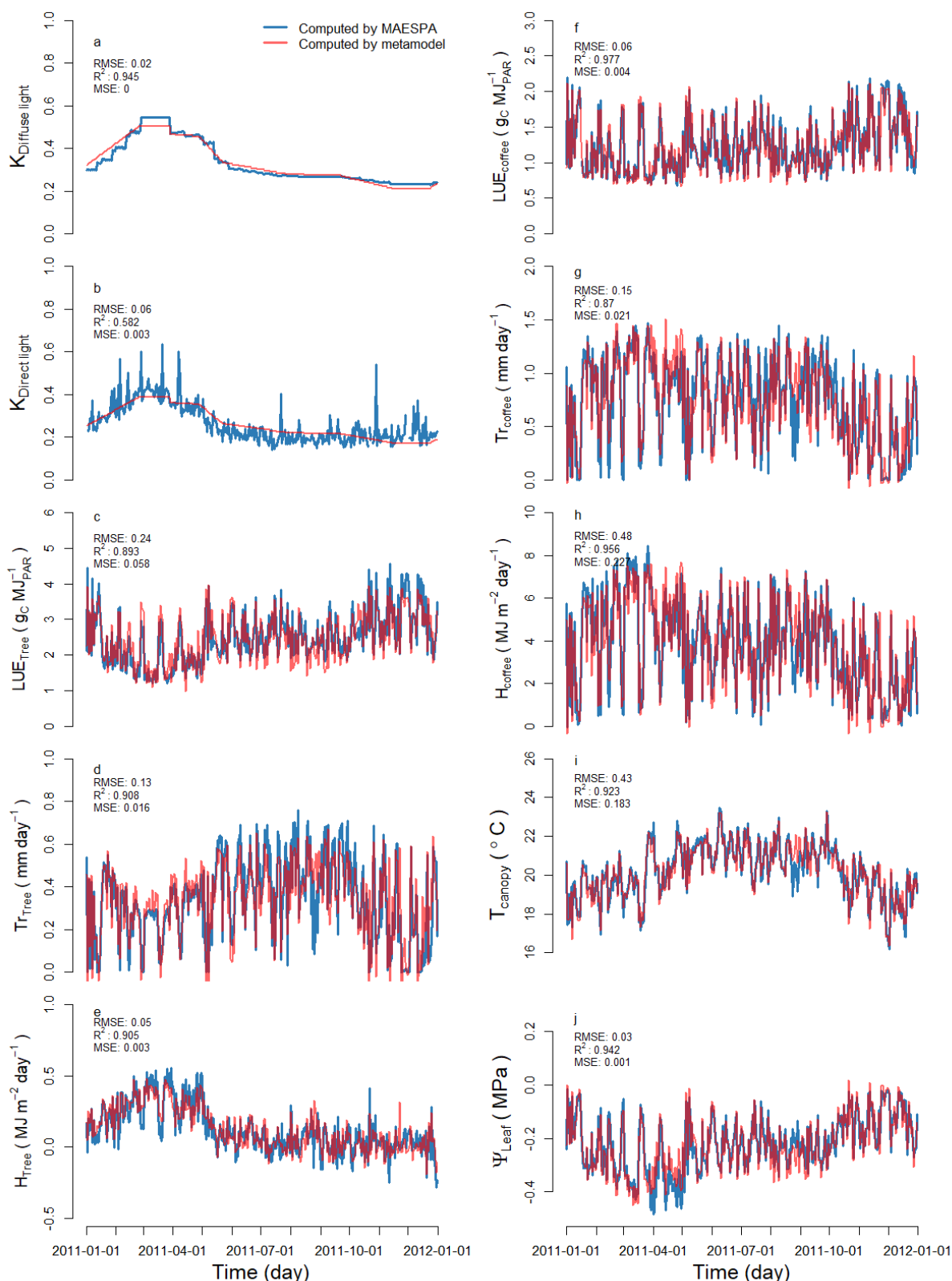
428 **Figure 18.** *Erythrina poeppigiana* shade tree main outputs along the full planting cycle. Trees were pruned twice a year before  
 429 2000 and then left free to grow. a/ LAI dynamic as compared to maximum and minimum recorded average in the litterature  
 430 denoted by the green rectangle. The minimum average is the mean – SE measured in 2011-2013 by Charbonnier et al. (2017b)  
 431 and the maximum average is the mean + SD value from Taugourdeau et al. (2014a), b/ shade tree light transmittance  
 432 compared to Charbonnier et al. (2013) mean and SD, c/ Stem and d/ branches carbon mass compared to Charbonnier et al.  
 433 (2017b) measurements.

434 The modelled coffee carbon allocation by organs showed that plant reserves represented by far the  
 435 compartment with the highest carbon flow, capturing in average 69% of the plant carbon offer, with a  
 436 maximum allocation to reserves of 80% of the daily offer, and a minimum of 0% during fruit production. This  
 437 compartment has also subjected to high turnover rate because reserves are almost directly re-allocated to  
 438 organs, making a yearly reserve balance close to 0 (Table 7). The leaves and branches were the organs with  
 439 the highest NPP, with 34.1% and 27.3% of the total yearly NPP respectively, because their carbon demand  
 440 was high, and it was almost always met. Fine roots represented, 16.3%, fruits 12.0% of total NPP, and stump  
 441 and coarse roots 10.3%.

442 Dynamic simulations were plotted for a full growing cycle from 1979 to 2016 in Figure 20, with  
 443 compartments following the allocation order. Resprout wood (Figure 19.a) grew rapidly from 0 to 6 YAP,  
 444 before the onset of the pruning cycle every 5 years which affected 20% of the resprouts of the plot population.  
 445 Under the pruning mode, resprout wood declined to reach a stable value of ca. 400 gC m<sup>-2</sup>, showing infra-  
 446 annual fluctuations, with growth before pruning and rapid drop after pruning. The behavior was different for  
 447 the perennial compartment of stump+coarse roots (Figure 19b) which was not subject to pruning: this  
 448 compartment grew approximately linearly until a maximum value of 1978 gC m<sup>-2</sup>, or 41.6 t<sub>DM</sub> ha<sup>-1</sup> at the end.  
 449 The coffee fruit compartment (Figure 19c) started to yield at 3YAP, reached its maximum values at young  
 450 ages, was affected by the pruning cycled starting from 6 YAP and declined to its stable values of around 50  
 451 gC m<sup>-2</sup>. It should be noted that the model did simulate the inter-annual fluctuations. The coffee leaf carbon  
 452 mass (Figure 19d) grew rapidly until reaching its maximum value of 181 gC m<sup>-2</sup> at four years old, and then  
 453 fluctuated between 119 and 161 gC m<sup>-2</sup> after pruning and until the end, corresponding to a LAI of 2.8 and 3.5  
 454 m<sup>2</sup> m<sup>-2</sup>. Fine roots (Figure 19e), like resprout wood grew rapidly in conjunction with LAI, but were impacted  
 455 right after the first pruning to reach a more stable, slightly decreasing state due to the combined effect of  
 456 pruning, natural mortality, and relatively decreasing carbon resources as the total plant maintenance  
 457 respiration grew with the increasing total plant carbon mass. The reserves compartment (Figure 19f)  
 458 fluctuated from season to season, mainly in opposition with the fruit carbon growth which is the last organ to  
 459 be filled before reserves: here the measured values correspond to a seasonal minimum measured once only, at  
 460 the time of grain-filling.

461 **Table 7. Dynamic crop model NPP simulation per organ and plant layer.**

Organ	Average NPP (gC m <sup>-2</sup> year <sup>-1</sup> ± SD)	
<i>Coffee</i> (Age > 5 years)		
Leaves	270 (1)	
Perennial wood (Stump + coarse roots)	81 (6)	
Branches	216 (31)	
Fine roots	129 (20)	
Fruits	95 (10)	
Reserve balance	0.05 (5.5)	
<i>Erythrina poeppigiana</i> shade tree	Pruned (1979-1999)	Free growing (>2000)
Leaves	9.7 (0.2)	76 (3)
Stem	4 (0.1)	33 (1)
Branches	7.6 (0.2)	58 (2)
Coarse roots	2.6 (0.1)	20 (1)
Fine roots	8.5 (0.2)	66 (3)

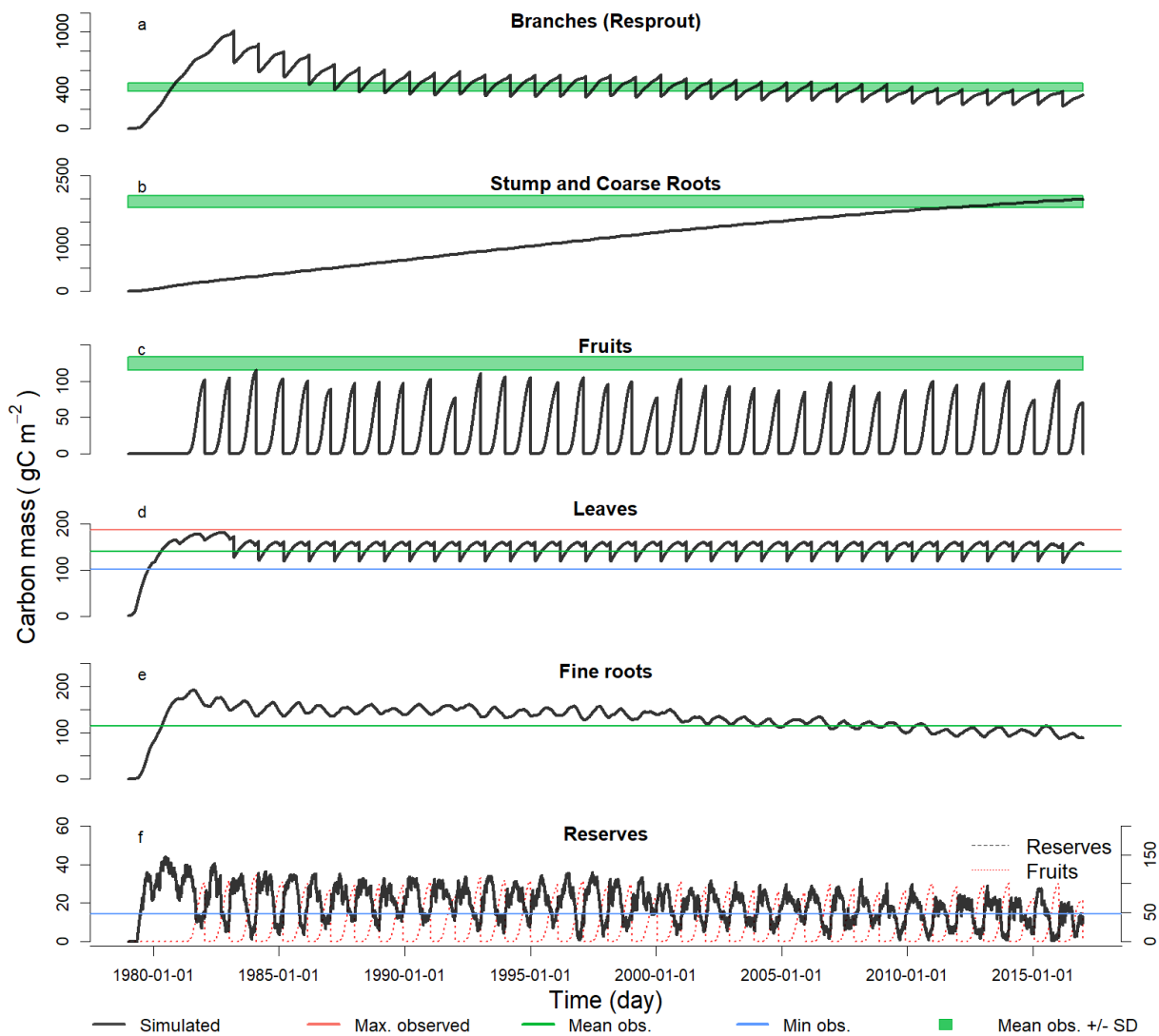


462

463 **Figure 19. a/ Shade tree diffuse and b/ direct light extinction coefficient, c/ Tree light use efficiency, d/ Tree transpiration, e/**  
 464 **Tree sensible heat flux, f/ Coffee light use efficiency, g/ Coffee transpiration, h/ Coffee sensible heat flux, i/ Coffee canopy**  
 465 **temperature and j/ Coffee leaf water potential, all computed by MAESPA model (blue) and by the subsequent metamodel**  
 466 **(red).**

467

468

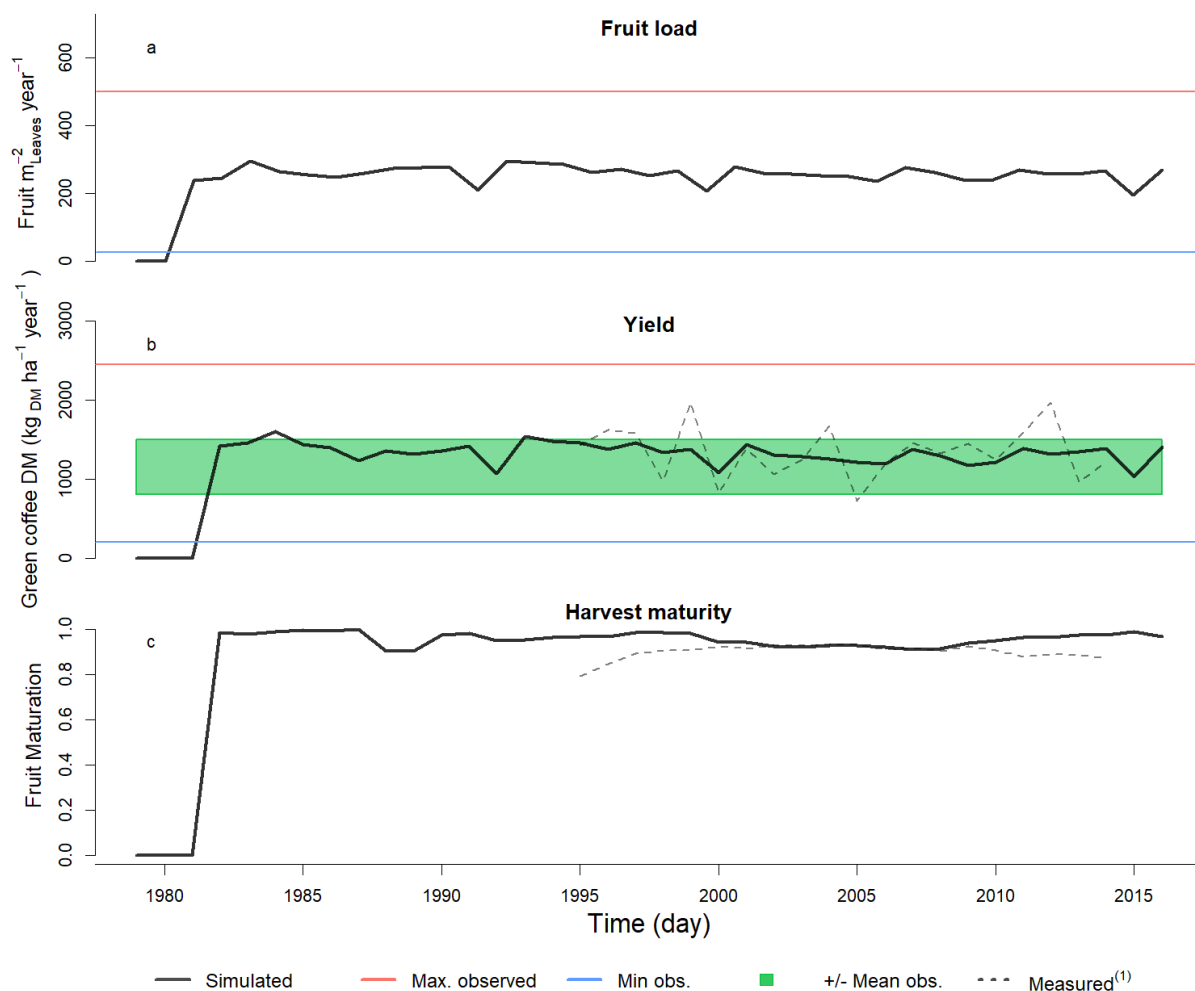


469

470 **Figure 20.** Coffee C biomass simulated (black lines) by organ throughout a full plantation cycle (1979-2016), compared to  
 471 measurements (colour lines) performed by the end of the cycle (2011 or 2012). a/ Simulated stump + coarse roots C biomass  
 472 (black line) compared to measured stump dry mass +/- SD in Charbonnier et al. (2017b) and measured perennial roots dry  
 473 mass found in Defrenet et al. (2016); b/ Simulated branches wood dry mass compared to Charbonnier et al. (2017b) measured  
 474 averaged +/-SE; c/ Simulated fruit dry mass compared to Charbonnier et al. (2017b) measurement values for 2011 and 2012 at  
 475 harvest (i.e. maximum of the year); d/ Simulated leaf dry mass compared to the mean value given by Charbonnier et al.  
 476 (2017b) on the same plot in 2011 (green line), and to the range of minimum and maximum values measured in Taugourdeau et  
 477 al. (2014a) between 2001 and 2011 in the same plot (blue and red lines, respectively); e/ Simulated fine roots C biomass  
 478 compared to Defrenet et al. (2016) measurement on the same plot in 2011; and e/ Simulated reserves compared to a  
 479 measurement made at the annual lowest expected value (after fruit production) in Cambou (2012) in blue line.

480 As soon as fruit buds appeared on coffee plants on the end of the third year (Figure 21), the modelled fruit  
 481 load reached a stable value around  $258 \text{ Fruits } m_{Leaves}^{-2} (\pm 23)$ . The dynamic crop model gave consistent  
 482 predictions in average compared to yield from close farms, with an average modelled green bean production  
 483 of  $1336 \text{ kg}_{DM} \text{ ha}^{-1} \text{ year}^{-1}$  against a measurement of  $1345 \text{ kg}_{DM} \text{ ha}^{-1} \text{ year}^{-1}$  between 1995 and 2014, but  
 484 it failed to reproduce some of the interannual variability, with a standard deviation of  $129 \text{ kg}_{DM} \text{ ha}^{-1} \text{ year}^{-1}$   
 485 only compared to  $339 \text{ kg}_{DM} \text{ ha}^{-1} \text{ year}^{-1}$ . Coffee beans maturity was always greater than 79%, with an  
 486 average of ca. 90%. It was found close to measurements between 2000 and 2009, but didn't catch the lower  
 487 maturity before and after this period.



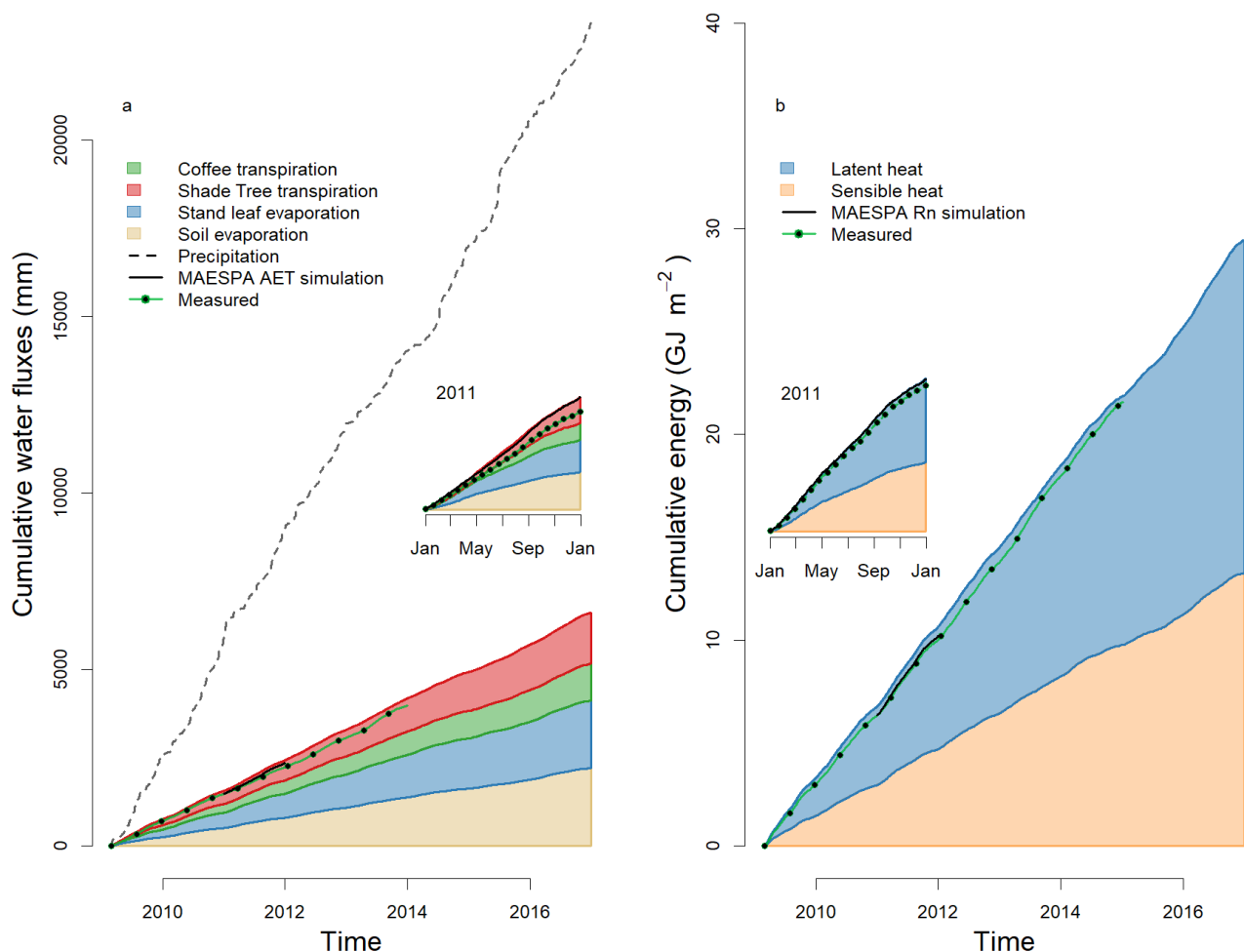


488

489 **Figure 21. Reproductive development of coffee.** a/ Fruit load compared to maximum and minimum observed in Charbonnier  
 490 et al. (2017b) in the same plot for years 2011-2013; b/ simulated yield compared to local measurements (dotted line), mean  
 491 yield (green rectangle) of the Central American countries (Söndahl et al., 2005), maximum (red line) observed in a  
 492 monoculture in Campanha et al. (2004) and minimum (blue line) generally observed (van der Vossen et al., 2015); c/ harvest  
 493 maturity compared to local measurements (dotted line). (1) Local measurements correspond to average values found in farms  
 494 near the simulated plot, with varying managements.

### 495 3.3. Water and Energy balance

496 The water and energy balance simulations by the crop model were compared to measurements from the long  
 497 term CoffeeFlux monitoring. As expected, the model outputs were very close to those from MAESPA in  
 498 2011. Indeed, both plants transpiration and sensible heat fluxes are computed using MAESPA metamodels,  
 499 and the soil energy partitioning between sensible and latent (*i.e.* soil evaporation) parameter was determined  
 500 thanks to MAESPA simulations. However, comparison with cumulated AET (Actual Evapo-Transpiration)  
 501 and net radiation measurements from the previous and subsequent years showed good consistency (RMSE:  
 502 AET= 0.56 mm, Rn= 1.55 MJ m<sup>-2</sup> day<sup>-1</sup>), confirming that the model still performs well outside of the  
 503 metamodel calibration year.



504

505 **Figure 22. Dynamic crop model simulation for cumulated a/ evapotranspiration and b/ energy partitioning along the 2009-2016**  
 506 **period. MAESPA simulation for AET (evapotranspiration) and Rn (net radiation) along the year 2011 as well as**  
 507 **measurements for the entire period are also presented for model assessment. Figures within the figures represent the**  
 508 **cumulative evapotranspiration and energy partitioning of the year 2011 only to better compare with MAESPA simulations (see**  
 509 **Vezy et al. (under review)).**

#### 510 4. Discussion

511 The dynamic crop model was rapidly developed and gave satisfactorily results thanks to the use of  
 512 metamodels from a more complex model, MAESPA. Hence, the resulting product consists in two different  
 513 kind of computations for its inner variables: the computation of metamodels that considers the spatial effect of  
 514 the shade tree canopy on light transmittance, light use efficiency, canopy temperature, transpiration, leaf water  
 515 potential and sensible heat flux; and the computation of the allocation of carbohydrates and the vegetative and  
 516 reproductive development of the coffee crop.

#### 517 4.1. Metamodels

518 The use of metamodels in dynamic crop models are promising, giving the possibility to implement complex  
 519 processes into simple models without the need of hard-coding them nor the expensive computation that often

520 comes along with them. Furthermore, physiological data are often sampled at leaf or plant scale, while  
521 dynamic crop models work at field scale. The use of MAESPA allowed to up-scale these fine-scale data to  
522 field scale for parameterisation while taking spatial anisotropy into consideration. Then, the MAESPA  
523 metamodels allowed the dynamic crop model to compute these plant-scale processes at plot-scale, and hence  
524 to better consider the continuous effect of shade on all these processes while a simpler plot-scale model would  
525 only consider shade effect as a constant (*e.g.* 30 % shade).

526 Therefore, LAD was found to predict well the light extinction coefficient ( $K$ ) of the shade tree layer, and  
527 hence its light absorption using its LAI. This result is consistent with the ones found in Sampson and Smith  
528 (1993) who determined the LAI and the foliage aggregation (clumping) as the most important characteristics  
529 for light penetration modelling. The clumping is likely species dependent, thus it can be expected that the  
530 metamodel for  $K$  may vary widely according to shade tree species. The use of metamodels allowed fast  
531 implementation of several spatial-dependant variables with low prediction error and fast computation. Being  
532 empirical, metamodels should be applied to new conditions with careful attention, because they tend to overfit  
533 their training data, and because complex metamodels can give unexpected results outside their training  
534 especially if they use non-linear fits. To overcome these aspects, the metamodels were trained and validated  
535 on different data, and were made using linear regression only. Marie et al. (2014) found that despite being  
536 slower to compute, neural networks and multi-linear regressions with two or three level interactions yielded  
537 higher  $R^2$  than multi-linear regressions with no interactions such as the ones used in our study. However,  
538 seven out of ten metamodels in our study gave  $R^2$  higher than 0.90 with low RMSE, which is considered as  
539 highly accurate, two gave  $R^2$  higher than 0.80, which is considered accurate (Villa-Vialaneix et al., 2012), and  
540 only one metamodel could be considered not sufficiently accurate with a  $R^2$  of 0.58.

541 Shade trees were pruned twice a year before 2000, making this period a new condition for the metamodels  
542 trained only in 2011 where trees grew freely. However, *E. poeppigiana* loses all its leaves once a year,  
543 therefore includes very low LAI in the training dataset. Indeed, the metamodel's simulated transmittance  
544 behaves well under pruning conditions, giving high values with low LAI, as well as the cumulated  
545 evapotranspiration and energy balance, which were satisfactorily predicted compared to measurements outside  
546 of their training period, even if both computations depended heavily on metamodels. The metamodel for the  
547 coffee LUE predicted an increase of LUE with a reduction of incoming radiation on the coffee layer, which is  
548 coherent with previous results, such as found in Charbonnier et al. (2017b).

549 Hence, metamodels allow overcoming the long-lasting trade-off between speed, accuracy, genericity, and fast  
550 development of dynamic crop models.

## 551 **4.2. Growth and yield outputs from the dynamic crop model**

552 Even if the site was well instrumented and documented for the last years of the coffee cycle, some lack of data  
553 still makes the dynamic crop model parameterisation difficult and the validation challenging for some  
554 processes. Our model has been subjected to a multi-objective validation against many different variables using

555 average measurements from the literature on other experiment, literature from the same experimental plot, as  
556 well as eddy-covariance measurements from the plot of interest. It should be noted that the model was  
557 empirically calibrated, and it probably could yield better results using parameter optimisation algorithm such  
558 as Bayesian calibration or evolutionary algorithms (Van Oijen et al., 2005). However, the model satisfactorily  
559 predicted most outputs with little or no discrepancy. The mean simulated leaf dry mass four years after  
560 planting ( $= 148.9 \text{ g}_C \text{ m}^{-2}$ ) was in agreement with the ones found in Charbonnier et al. (2017), Taugourdeau et  
561 al. (2014) and Siles et al. (2010), with values of 140.5, 143.7 and from 102 to  $176 \text{ g}_C \text{ m}^{-2}$  respectively. Well  
562 predicting the leaf dry mass is of high importance in dynamic crop models because it leads all further  
563 computations through photosynthesis and transpiration. The seasonal behavior of leaf biomass showed a drop  
564 by the end of the dryer season corresponding to natural leaf shedding followed by pruning, increased rapidly  
565 at the beginning of the rainy season and expressed a secondary minimum at the time of grain-filling.  
566 Interestingly, the simulations mimic well the seasonal observations reported by Taugourdeau et al. (2014) and  
567 the average is close to measured values. Such a strikingly realistic seasonality was achieved only after we  
568 introduced fruit cohorts into the code: without explicit fruit cohorts in the model, all fruits ripened at the same  
569 moment, creating a huge C demand at the time of grain-filling, leading to an unreasonable LAI drop at the  
570 time of grain filling (no more leaf growth, continued leaf mortality). After distributing the fruit demand into  
571 cohorts, the LAI drop was visible but just moderate during the grain-filling and corresponded precisely to  
572 observations (Taugourdeau et al., 2014). However, to date, the simulated magnitude remains lower than  
573 observed and the simulated interannual variability is hardly perceived, whereas it can be large in field  
574 conditions. We assume that some processes driving the interannual variability of LAI are still to be  
575 implemented into the model, through (i) a variable leaf lifespan according to the season and (ii) a variable  
576 mortality due to leaf diseases. Indeed, we included a model for American Leaf Spot (ALS) here, following  
577 Avelino et al. (2007), but the main leaf disease affecting this area is coffee leaf rust and is not implemented  
578 yet due to the absence of published empirical model linking severity and leaf losses.

579 Perennial wood NPP, taken as the sum of stump, coarse roots and resprout wood was found underestimated by  
580 20% compared to Charbonnier et al. (2017), but their total carbon mass was satisfactorily simulated in the end  
581 of the simulation. This probably comes from an underestimation of the NPP, followed by a lower mortality  
582 compared to reality. The total aboveground carbon mass of the agroforestry system fell within the range given  
583 in Charbonnier et al. (2017) for both 2012 and 2013. Interestingly, we obtained a reasonable prediction of  
584 stump+coarse root dry mass by the end of the cycle only after changing the allocation coefficient to this  
585 compartment according to the age of the coffee plant: indeed, we had to allocate more C to this compartment  
586 for older plants, which sound rather counter-intuitive but was actually reported in Defrenet et al. (2016). They  
587 found that the ring width increased from year 1 to year 12 and then remained constant around 2 mm per year  
588 after 12 YAP. This implies that allocation increases with time to sustain the increasing wood mass  
589 accumulation per year. Once implemented into the model, this observation allowed balancing most  
590 compartments during the multi-objective calibration process.

591 One particularly interesting organ to compare is the fruit yield because its allocation follows a complex  
592 scheme that is inspired from Rodríguez et al. (2011). Well predicting this compartment is challenging because  
593 it is a two-year process (Camargo and Camargo, 2001) that depends on many factors. The predicted yield was  
594 within the range of the national average productions in Central America given in Söndahl et al. (2005), but  
595 was only 80 and 70% of the yield measured in Charbonnier et al. (2017) at plot scale for 2012 and 2013  
596 respectively. However, our model was more in agreement when compared to resprout-scale measurement  
597 from 2013 in the same study, with 106% of the measurement. Furthermore, a comparison with average  
598 measurements from farms close to the simulated point showed that the model is more able to reproduce the  
599 average production trend (measured average:  $1345 \text{ kg}_{DM} \text{ ha}^{-1}$ , simulated:  $1313 \text{ kg}_{DM} \text{ ha}^{-1}$ ) than its  
600 variability (measured SD:  $339 \text{ kg}_{DM} \text{ ha}^{-1}$ , simulated:  $129 \text{ kg}_{DM} \text{ ha}^{-1}$ ). Again, the interannual variability  
601 seems to be underestimated by the model and this might be linked with leaf diseases for instance. Therefore,  
602 the model can be an efficient tool to predict tendencies of productions in response to climate and management,  
603 more than a tool that predicts the exact yield of a particular plot in a particular year.

604 The shift in tree management from pollarded to free-growing seemed to have little impact on fruit production  
605 or quality. This apparent stability came from the low density of the shade trees, which still transmitted 86% of  
606 light at mature state, Charbonnier et al. (2017) reported that the higher LUE simulated by MAESPA for coffee  
607 plants under higher shade could compensate a large part of the decreased incident PAR, maintaining NPP at a  
608 nearly-constant level. Indeed, GPP decreased only slightly as compared to a constant LUE.

609 Another capacity of the model is to predict water and energy balance thanks to the full implementation of the  
610 BILJOU model and to the MAESPA metamodels. Indeed, predictions of the cumulated AET and net radiation  
611 were very close the continuous measurements between 2009 and 2015.

612 A model is first made to resemble reality, and can then be used to better understand it. Therefore, assuming  
613 the model gave satisfactorily results, it can provide further information that was not apparent from the data.  
614 Indeed, coffee LAI is strongly affected by pruning once a year and in between by natural mortality and fruit  
615 demand at the time of grain filling for years of high fruit load, which was also observed by Charbonnier et al.  
616 (2017). Another effect observed in model outputs is that except for stump and coarse roots which are the only  
617 perennial compartments, biomass increases rapidly at the early stages of the plantation until its maximum  
618 value over the rotation, and then biomass growth starts decreasing with pruning, and finds a new and lower  
619 equilibrium between growth and natural and pruning mortality. Yield is maximum in the first stages of the  
620 plantation, as observed in the field, then decreases gradually with age, even under full sun management (not  
621 shown). A last point to consider is that the model does not reproduce the so-called fruit biennial production  
622 (Cannell, 1985b), but as Van Oijen et al. (2010b) already stated for their model predictions, it is believed that  
623 this phenomenon vanishes at plot-scale due to the heterogeneity in the age of the resprouts: indeed bienniality  
624 is rather visible either at the plant scale, or for equiennial resprouts, notably during the first years after  
625 planting.

## 626 **5. Conclusion and outlook**

627 A dynamic crop growth and yield model has been developed to simulate coffee plantations under different  
628 possible managements. The management can be set as any shade type and density, from full sun to multi-  
629 species (i.e. multi-strata) agroforestry systems, applying pruning or thinning at any age if required. The model  
630 can be used for full rotations at daily time-step to any number of points, from a plot to regions or even more,  
631 under current, past or future climate as soon as the metamodels, build from MAESPA 3D model simulations,  
632 are updated to the conditions in use. The model has been parameterized using state-of-the-art parameters and  
633 calibrated on a comprehensive and unique dataset for energy and water balance, biomass and NPP. The model  
634 was then checked using a multi-objective validation on the database and available literature. Other data  
635 remain limited, especially under agroforestry management, but being a tree-average plot model, the  
636 calibration can be made using plot averages or totals which are more frequently available from farms (e.g.  
637 yield, pruning intensity, coffee quality...). Another important feature of the model is the cohorts of flowers  
638 and fruits that were implemented to encompass grouped flowering situations as in sub-tropical conditions to  
639 distributed as in equatorial climate. The model being coded in R, it is also made for easy sharing and  
640 collaboration, and is flexible enough to be easily modified to add new modules as pests, nutrient cycling,  
641 SOM or soil respiration. The methodology can be further generalized for any type of shade or climate by  
642 using different MAESPA simulation sets for metamodels training, in order to apply the dynamic crop model  
643 on future climate predictions under different management scenarios.

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- 784

### 3.4. Conclusion du chapitre

Un modèle dynamique de culture a été développé pour simuler les plantations de café sous différentes gestions possibles, et différents climats. L'utilisation de métamodèles issus de MAESPA nous a permis d'intégrer rapidement à notre modèle dynamique des processus complexes liés à la gestion du café en agroforesterie tels que les effets anisotropiques de température, d'interception lumineuse et d'humidité de l'air. Ceci nous a permis de nous concentrer sur l'intégration d'autres processus novateurs, tels que la production de cohortes de fleurs et de bourgeons, l'avortement des fleurs, la dormance des bourgeons, ou encore le remplissage et la maturation des fruits.

La gestion peut être définie dans le modèle comme n'importe quel type d'ombrage et de densité, allant des systèmes de cultures en plein soleil à des systèmes agroforestiers multi-espèces (c'est-à-dire multi-strates), tout en appliquant des interventions tels que de l'élagage ou de l'éclaircissement à n'importe quel âge si nécessaire. Le modèle peut être utilisé pour des rotations complètes au pas de temps journalier sous climat actuel, passé ou futur tant que les métamodèles issus de MAESPA sont entraînés sur ces conditions. Le modèle a été paramétré selon l'état des connaissances actuelles, et étalonné sur un ensemble de données unique pour les bilans d'énergie et d'eau, la biomasse et la production nette de carbone. Le modèle a ensuite été testé en utilisant une validation multi-objectif sur des données mesurées ou issues de la littérature. Etant un modèle à l'échelle de la parcelle, le paramétrage peut être effectué en utilisant des moyennes parcellaires, qui sont plus facilement disponibles depuis les exploitations agricoles (*e.g.* les rendements, l'intensité d'élagage, la maturité des grains...). Une autre caractéristique importante du modèle est l'intégration de cohortes de fleurs et de fruits, qui ont été développées pour prendre en compte les régimes de floraison groupés ou étalés selon les conditions climatiques. La méthodologie peut être généralisée pour tout type de gestion ou de climat en utilisant différents jeux de simulations pour l'entraînement des métamodèles de MAESPA.

C'est ce que nous faisons dans le chapitre suivant, dans lequel nous appliquons le modèle sur des prédictions climatiques futures pour deux sites, et sous différents scénarios de gestion.



# **Chapitre 4. Modelling *Coffea arabica* adaptation to future climate change: neither CO<sub>2</sub> nor shade remediate projected yield losses at low elevations.**

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## 4.1. Introduction au chapitre

Ce chapitre est la suite directe du troisième chapitre, qui a pour objectif d'utiliser le modèle sur des projections climatiques sur le même site agroforestier sur lequel il a été précédemment testé (Aquiaries), ainsi que sur un autre site plus en altitude au Costa Rica, Tarrazu, qui est réputé pour son café de qualité. Ce chapitre a aussi pour objectif de tester plusieurs gestions d'arbres d'ombrage comme levier d'adaptation de la culture du café aux futurs climats, ainsi que tester les effets de l'augmentation de la concentration en CO<sub>2</sub> atmosphérique et de la température séparément.

## 4.2. Résumé en français

Les changements climatiques vont probablement affecter la production de café arabica, mais il est encore incertain de quand et comment elle sera impactée, car des interactions complexes de processus sont à l'œuvre. L'agroforesterie est déjà utilisée pour atténuer les extrêmes climatiques dans les cultures de café, et pourrait être utilisée pour adapter les cultures à l'augmentation de la température de l'air provenant des changements climatiques. Cependant, l'ajout d'arbres d'ombrage réduit la photosynthèse des caféiers à cause de la réduction de lumière transmise, mais l'augmentation de la [CO<sub>2</sub>] pourrait aider à compenser cet effet négatif. La modélisation des processus écophysologiques, basée autant que possible sur une représentation mécaniste, peut aider à mieux comprendre les différentes interactions des effets en jeu, et ainsi aider à mettre en place des moyens d'adapter la gestion pour compenser les futurs effets néfastes des changements climatiques. Cependant, jusqu'à présent aucun modèle n'incorpore les effets de la température sur la phénologie de la reproduction du café dans les AFS comme mécanisme. Un nouveau modèle de dynamique de culture a été couplé à un modèle 3D grâce à l'utilisation de métamodèles pour étudier les interactions spatiales complexes entre la lumière interceptée, l'efficacité de l'utilisation de la lumière, le CO<sub>2</sub>, et la température de 1979 à 2099. Les simulations ont montré que l'augmentation de la température seule à l'horizon 2100 aurait un effet négatif sur la NPP du café (-11.2%), mais que l'effet positif de l'augmentation de la concentration en CO<sub>2</sub> atmosphérique dépasse cet effet négatif de la température, résultant en une plus grande NPP (+25.5% avec les deux effets). De plus, les simulations montrent que les arbres d'ombrage ont un effet de plus en plus positif sur le rendement du café sous les climats futurs comparé au café cultivé en monoculture, jusqu'à +20.9% sous RCP8.5. Ce phénomène est particulièrement vrai lors d'une adaptation progressive de la gestion des arbres d'ombrage via l'éclaircissage et l'émondage. Cependant, il est important de noter que le modèle prédit que ni le CO<sub>2</sub>, ni l'ombrage ne peuvent aider à maintenir les rendements actuels des caféiers à l'horizon 2100, quel que soit le site ou la gestion.

1 4.3. Article scientifique

2 **Modelling *Coffea arabica* adaptation to future climate change:**  
3 **neither CO<sub>2</sub> nor shade remediate projected yield losses at low**  
4 **elevations**

5 Rémi Vezy<sup>a,b,c\*</sup>, Olivier Roupsard<sup>a,b,d</sup>, Selena Georgiou<sup>d</sup>, Pablo Imbach<sup>d</sup>, Bruno Rapidel<sup>d,e</sup>, Fabien Charbonnier<sup>a,b,f</sup>, Céline  
6 Blitz-Frayret<sup>a,b</sup>, Denis Loustau<sup>c</sup>, Hugo G. Hidalgo<sup>g,h</sup>, Eric J. Alfaro<sup>g,h</sup>, Gueric le Maire<sup>a,b,i</sup>.

7  
8 <sup>a</sup>CIRAD, UMR Eco&Sols, F-34398 Montpellier, France.

9 <sup>b</sup>Eco&Sols, Univ Montpellier, CIRAD, INRA, IRD, Montpellier SupAgro, Montpellier, France

10 <sup>c</sup>INRA, UMR 1391 ISPA, F-33140 Villenave d'Ornon, France

11 <sup>d</sup>CATIE, Centro Agronómico Tropical de Investigación y Enseñanza, Turrialba 30501, Costa Rica

12 <sup>e</sup>CIRAD, UMR System, 34060 Montpellier, France

13 <sup>f</sup>El Colegio de la Frontera Sur, CONACyT research fellow, San Cristóbal de las Casas, 29290 Chiapas, México

14 <sup>g</sup>Escuela de Física, University of Costa Rica, 2060-Ciudad Universitaria Rodrigo Facio San Pedro, San José, CR.

15 <sup>h</sup>Center for Geophysical Research, University of Costa Rica, 2060-Ciudad Universitaria Rodrigo Facio San Pedro.

16 <sup>i</sup>UNICAMP, NIPE, Campinas, Brazil

17 \*Corresponding author. Email address: remi.vezy@cirad.fr (R. Vezy).

18

19 **Abstract**

20 *Coffea arabica* bean production will be affected by climate change, with probable decrease, but it is unknown  
21 how and when yield will be impacted because complex interactions of processes will occur. Agroforestry is  
22 already used to buffer high air temperature in coffee crops, and could be used to attenuate the negative effect  
23 of high temperature under future climate. However, a major trade-off is that addition of shade trees also  
24 decreases the incoming light for the coffee layer growing below, which reduces its photosynthesis. But the  
25 increasing [CO<sub>2</sub>] could help compensating for this negative effect. Ecophysiological process modeling based  
26 as much as possible on mechanistic representation of the processes may help disentangle the different effects,  
27 and eventually help finding ways for adapting the management to counterbalance future adverse effects of  
28 climate changes. However, no model incorporated effects of temperature as a mechanism on the reproductive  
29 phenology of coffee in AFS so far. Such an original dynamic crop model was coupled to a 3D model through  
30 metamodels, to study the complex spatial interactions between intercepted light, light use efficiency, CO<sub>2</sub>, and  
31 temperature from 1979 until 2099. The simulations showed that increased temperature had a negative effect  
32 on coffee NPP by horizon 2100 (-11.2% alone), but that increased CO<sub>2</sub> concentration had a positive effect that  
33 exceeded the temperature effect (+25.5% with both effects). Shade trees had an increasingly positive effect on  
34 coffee yield under future climate compared to coffee grown in monoculture, up to +20.9% under RCP8.5.  
35 This was particularly the case with a progressive adaptation of the shade tree management such as thinning  
36 and pruning. However, neither CO<sub>2</sub> or shade could help sustain current coffee yield in any sites or  
37 managements by the 2100 horizon.

38 **Keywords:** dynamic crop model; process-based model; MAESPA; metamodel; yield; climate change;  
39 adaptation; agroforestry; *Coffea arabica*.



## 40 1. Introduction

41 Current knowledge on climate change effects on agronomic systems are still uncertain due to different  
42 climatic projections and spatial or temporal scale effects. Indeed, whereas air temperature and CO<sub>2</sub>  
43 concentration are likely to increase everywhere in the tropics and rainfall trends may depend on the regions,  
44 climate changes effects on agronomic systems will probably depend on local conditions and crop types.  
45 Indeed, each crop has its own environmental optimum with different ranges of temperature, vapor pressure,  
46 precipitations, or nutrients. Beyond this range, crops can rapidly become unsustainable and must be either  
47 adapted or replaced. For fruit crops, the reproductive phenology and its sensitivity to climate factors is  
48 generally poorly known and biases the predictions. There are several ways to adapt crops to new conditions,  
49 but most options are based upon existing practices and sustainable management rather than exclusively new  
50 technologies (Jarvis et al., 2011). Depending on the pace of climate changes and the crop under consideration,  
51 several adaptation strategies can be applied. Genetic improvements form part of the solution to mitigate  
52 impacts in annual species, but are less suited for long-rotation species used in tree-based agriculture and  
53 silviculture. Management can also be modified to adapt the crop. For example, annual crops can be sowed  
54 earlier to avoid the heat wave or the driest season, or planted under shade trees in agroforestry systems to  
55 buffer the micro-climate variations (van Noordwijk et al., 2014). Agroforestry also has many other benefits,  
56 such as a better control of pests and diseases, enhanced ecosystem services, better drought tolerance and  
57 higher and more stable income value (Malézieux et al., 2009; Verchot et al., 2007), but tend to complexify the  
58 system, and make management decisions more challenging.

59 *Coffea arabica* is a good candidate to study climate change impacts on complex crop structures. Indeed,  
60 coffee can be grown either in monoculture or under agroforestry systems. It is a widely exchanged product,  
61 has high world export value 27.2 BUS\$ (Comtrade, 2013), and is mainly produced by smallholders (70% of  
62 the world's coffee, (Kolk, 2013; Morris et al., 2016)). Two major species are cultivated for coffee beans  
63 production: *Coffea arabica* which is grown on mountains, and *C. canephora* on lowlands. *Coffea arabica*  
64 represents approximately 56% of global production and is renowned for its high gustative quality (Cagliani et  
65 al., 2013). As Coffee plantations have long life cycles of approximately 40 years, stakeholders need insights  
66 on possible climate change impacts on coffee production to adapt their plantations from planting. Basing on  
67 suitability models only, it has been argued already that *C. arabica* is highly sensitive to climate changes and  
68 that global warming will threaten the whole coffee supply in the near future (Davis et al., 2012; Bunn et al.,  
69 2015), mainly because of the temperature rising, as its optimal annual mean temperatures for development are  
70 between 18 and 23°C (DaMatta and Ramalho, 2006). Furthermore, there is a general belief that the coffee  
71 production has already been affected by climate changes in several coffee-growing countries, especially by  
72 adverse events associated with severe drought periods in combination with high temperatures (Bunn et al.,  
73 2015; van der Vossen et al., 2015). Furthermore, modeling studies have even foreseen dramatic effects of  
74 climate changes on the coffee crop, including significant changes in agro-climatic zoning, loss of suitable  
75 areas in the largest coffee-producing countries such as Brazil or Vietnam (Assad et al., 2004; Zullo Jr et al.,

76 2011;Bunn et al., 2015), productivity reductions (Gay et al., 2006;Bunn et al., 2015;Craparo et al.,  
77 2015;Ovalle-Rivera et al., 2015), wild populations of *C. arabica* extinctions (Davis et al., 2012) and increased  
78 agricultural, social and economic vulnerabilities (Baca et al., 2014). Coffee yield could be increasingly  
79 affected by climate change intensity through flower abortion or malformation. Indeed, daily average air  
80 temperature higher than 20.5°C (23°C and 18°C for day and night temperature respectively) could lead to a  
81 decrease of flower numbers, while abnormal flower types (Estrella) would appear beyond 25.5°C (28/23°C  
82 amplitude) and flowering disruption around 30.5°C (Drinnan and Menzel, 1995;Rodríguez et al.,  
83 2011;Ramírez, 2009).

84 However, thanks to its capacity to reduce air temperature and to optimize incident light for coffee flowering  
85 on highly managed plantations, growing coffee under shade trees has been a traditional solution for less-  
86 favorable environments like lowland productions (DaMatta, 2004), and even sometimes under optimal  
87 conditions (Siles et al., 2010). Therefore, agroforestry could be used as a tool to adapt coffee plantations to the  
88 increasing air temperature of the near future. However, despite its buffering effect on microclimatic conditions  
89 (Lin, 2007), shade decreases the incoming light on the coffee layer, which could reduce photosynthesis. Yet, it  
90 has been shown that coffee light use efficiency (LUE) increase under shade and compensate the reduction of  
91 light to some extent on coffee net primary productivity (NPP), at least moderate shade tree density  
92 (Charbonnier et al., 2017). Although coffee carbon balance could be negatively impacted beyond optimal  
93 temperature through increased maintenance respiration and decreased photosynthesis and negative effects on  
94 the reproductive phenology, CO<sub>2</sub> fertilization could enhance photosynthesis, and possibly compensate such  
95 effects (Rodrigues et al., 2016;Ghini et al., 2015). This could allow higher shade tree densities for temperature  
96 regulation to sustain the number of flowers, while avoiding a collapse of the carbon balance. In other words,  
97 stakeholders could increase shade trees density to sustain current coffee carbon production ranges in future  
98 conditions. Yet, we argue that there is no field experiment available so far to document the effects of both  
99 CO<sub>2</sub> and temperature on the reproductive phenology of Arabica. Hence, numerical models for a fruit crop  
100 such as coffee should be based on all the reproductive phenology available to date.

101 To disentangle this complex task, we used a modelling scheme presented in Vezy et al. (in prep.). Indeed,  
102 accurate light interception modelling in complex canopies such as coffee agroforestry systems requires 3D  
103 explicit models. However, these models are often time-consuming for plant to plot scale computations,  
104 making them unsuitable to simulate growth and yield predictions over several managements and long-time  
105 periods. Thus, the dynamic crop model in use was coupled to a 3D process-based model through simple  
106 metamodels to compute all spatial-dependent variables such as light interception, light use efficiency,  
107 transpiration, or canopy temperature. The coffee growth is then computed using allocations rules for each  
108 compartment, considered at the plot-scale, and the reproductive development is computed using cohorts of  
109 buds and fruits following Rodríguez et al. (2011) and Drinnan and Menzel (1995), considered here as the  
110 finest information available so far to link reproductive phenology with temperature. Several experimental  
111 results on *C. arabica* sensitivity to microclimate are available. However, we argue that the experimental

112 information remains incomplete so far. Drinnan and Menzel (1995) studied the reproductive phenology  
113 according to temperature and showed that the number of flowers, thus yield was affected beyond a threshold.  
114 Ghini et al. (2015) showed that Arabica yield was enhanced under high CO<sub>2</sub> concentrations in a FACE  
115 experiment, but there were no temperature treatments so the interaction between CO<sub>2</sub> and temperature remains  
116 unknown. Rodrigues et al. (2016) showed in [CO<sub>2</sub>] x Temperature climate chambers that leaf photosynthesis  
117 was affected by high temperature, and that high [CO<sub>2</sub>] could compensate this effect: unfortunately, there was  
118 no information on allocation and reproductive phenology. Therefore, we argue that the community still misses  
119 crucial experimental evidences of the interactions between [CO<sub>2</sub>] and temperature on yield.

120 Coffee process modeling attempts were also developed in parallel: Van Oijen et al. (2010b) proposed a plot-  
121 scale multipurpose agroforestry model designed for climate change simulations, but the allocation and  
122 reproductive phenology had little experimental basis at that time and there was no continuous light gradient  
123 between shaded and non-shaded plots as stressed as an important factor by Charbonnier et al. (2013).  
124 Rodríguez et al. (2011) proposed a refined allocation and reproductive coffee model at the plant scale and in  
125 full sun, but shade and microclimatic effects were not incorporated into this model so far. Vezy et al. (in prep.)  
126 combined the reproductive phenology module of Rodríguez et al. (2011) and temperature sensitivity of  
127 flowers of Drinnan and Menzel (1995) into a new coffee agroforestry model based on Charbonnier et al.  
128 (2013), including the compensating effect of shade on coffee light-use efficiency reported in Charbonnier et  
129 al. (2017): however, this model was tested only on one coffee plot so far, with much details on NPP and  
130 allocation and no attempt was made to test it under climate change scenarios.

131 Consequently, the purpose of this study is to investigate through process based modeling the effects of future  
132 climate change of three factors, and their interactions on coffee production: (1) the temperature increase, (2)  
133 the atmospheric CO<sub>2</sub> concentration increase and (3) the change of shade quality through various management  
134 scenarios. The underlying hypothesis are that air temperature rise will increase maintenance respiration and  
135 photosynthesis, and reduce the number of flowers per plant (Drinnan and Menzel, 1995), and thus probably  
136 negatively impact coffee production. However, shade tree type and density could help reducing the coffee  
137 canopy temperature (Vezy et al., under review), help sustaining the number of flowers and consequently the  
138 yield, while increased LUE under shade trees and CO<sub>2</sub> fertilization could partially or entirely compensate the  
139 NPP decrease due to the decrease of incident light above the coffee layer. Our study could bring to light the  
140 possibility to sustain coffee production to the current level thanks to shade management and elevated  
141 atmospheric CO<sub>2</sub> concentrations, and thus orient the coffee adaptation research not only towards genetic  
142 adaptation, but also towards shade management changes in order to help stakeholders in their management  
143 decisions.

## 144 2. Materials and methods

### 145 2.1. Study sites and climate projections

146 Two locations of contrasted elevation and climate in Costa Rica were used for coffee stand simulations under  
147 different climate projections. Tarrazu is under pacific influence with seasonal drought and at high elevation  
148 (ca. 1500 m.a.s.l) while Aquiares is at lower elevation (1040 m.a.s.l) and under Caribbean influence, which  
149 results on higher precipitations. More details on the Tarrazu site can be found in Meylan et al. (2013) and  
150 Meylan et al. (2017), and on the Aquiares site in Gómez-Delgado et al. (2011), Benegas et al. (2014) or  
151 Taugourdeau et al. (2014).

152 Monthly average prediction from 20 GCM projections that were statistically downscaled to the point  
153 following Hidalgo et al. (2016) methodology from 1979 until 2100, for two representative concentration  
154 pathways (RCP):  $+4.5 W m^{-2}$  and  $8.5 W m^{-2}$ . The monthly averaged predictions of air temperature ( $^{\circ}C$ ),  
155 relative humidity (%) and precipitations (mm) from the downscaled GCM projections ( $MA_{GCM}$ ) were then  
156 transformed to a 30-minute time-step dataset using the variability of 4-year of continuous meteorological  
157 measurement (2009-2013) at each site. First, each month of the period was randomly associated to one of the  
158 same months among the four years of in-situ measurements, to form a dummy 30-minute dataset of air  
159 temperature ( $^{\circ}C$ ), relative humidity (%), photosynthetic active radiation ( $W m^{-2}$ ), global radiation ( $W m^{-2}$ ),  
160 windspeed ( $m s^{-1}$ ) and air pressure (hPa). Then, the future trend of each variable in the GCM projections were  
161 adjusted by computing the monthly ratio  $r$  of the GCM to the dummy time series. Finally, the monthly  $r$  value  
162 was multiplied with the dummy variable to create a 30 minutes dataset with the same GCM trends but with  
163 hourly and daily variations. The vapor pressure deficit (VPD) was generated from the newly generated air  
164 temperature and relative humidity.  $CO_2$  concentrations were downloaded from the official CMIP5  
165 recommended data RCP Database V2.0 (Meinshausen et al., 2011).

### 166 2.2. Coffee management

167 Currently, stakeholders in Costa Rica extensively use agroforestry systems for coffee production, with a wide  
168 range of shade species (Banana, *Cordia alliodora*, *Erythrina poeppigiana*, *Chloroleucon eurycyclumn*,  
169 *Terminalia amazonia*...), shade management intensity varying from highly pruned to free growth. They  
170 normally use fertilizer in excess but do not irrigate, and we will assume in the following model that nutrients  
171 are non-limiting, contrary to water. Among these, three contrasted shade management were selected in the  
172 present study to represent the wide variety of possible managements (Table 8): a coffee plantation in  
173 monoculture, subsequently referred as Full Sun, a coffee plantation in agroforestry management under free  
174 growing *Cordia alliodora* shade trees (Cordia), and under pruned *Erythrina poeppigiana* (Erythrina). *C.*  
175 *alliodora* is a fast-growing tree with high cover potential which grows freely to ca. 30 meters high and is used  
176 for timber. It is planted at low densities and is generally depressed when its canopy intercepts more than 30%

177 of total light (*i.e.* transmittance lower than 0.7) to avoid overly shaded conditions and to dispatch revenue  
178 from timber. *E. poeppigiana* is from the *Fabaceae* family, and is planted at high densities while pruned twice  
179 a year to optimize light conditions for coffee plants and to fertilize the soil with organic matter and nitrogen.  
180 Different set of management were tested on the three growing cycles to uncover the potential effect of shade  
181 on coffee bean production. Cordia shade management was tested with different starting tree densities (*e.g.*  
182 from reference 50 to 100 trees ha<sup>-1</sup>) and different thresholds of lowest transmittance before thinning (*e.g.* 0.2  
183 to the reference 0.7). The reference Erythrina management with two pruning a year is designed to optimize the  
184 light incoming to the coffee layer, with higher shade during bud initiation and fruit growing, and lower shade  
185 during vegetative development. However, the increased future changes of air temperature due to climate  
186 change will impact the timing of the coffee development stages along the year, making the reference  
187 management of shade trees not optimum for buds and fruits development if fixed dates of Erythrina pruning  
188 were kept. Therefore, Erythrina management was tested with different planting densities (*e.g.* from the  
189 reference 200 to 400 trees ha<sup>-1</sup>), and with or without pruning during the bud initiation. To prevent analyzing  
190 unrealistic shade management, preliminary tests were performed, and the shade management practices which  
191 gave very high drops of yield compared to Full Sun were not kept as potential management scenarios and  
192 discarded from the analysis. For example, this was the case for Cordia shade management with a late thinning  
193 keeping transmittance lower than 20%. Furthermore, Cordia management was also tested using several  
194 densities at planting (50, 75 and 100 trees ha<sup>-1</sup>). Comparing plots with the same transmittance threshold for  
195 thinning but different planting densities showed that plots with higher densities were more thinned in the  
196 beginning than plots with lowest densities. This difference in the thinning rate made all plots quickly converge  
197 to the same density values after few thinning events. Therefore, only one planting density was kept for all  
198 Cordia simulations: the reference 50 trees ha<sup>-1</sup>.

### 199 **2.3. MAESPA metamodels**

200 MAESPA is a tree-scale process-based model (Duursma and Medlyn, 2012) that computes flows of energy,  
201 water and carbon at voxel level. Each voxel is a homogeneous representation of a part of the tree crown from  
202 a particular species that has a set of physical properties such as a leaf area, a leaf angle, light transmittance,  
203 absorption and reflectance, and physiological properties such as stomatal conductance, photosynthetic and  
204 maintenance respiration parameters. The voxel level simulation is then upscaled to the tree scale, and then to  
205 the plot scale by coupling the plant and soil fluxes balance. This 3D integrating scheme is well suited for  
206 heterogeneous canopy modelling such as agroforestry systems, because it accounts for light anisotropy that  
207 leads all ecosystem processes such as photosynthesis, transpiration, evaporation, and canopy temperature  
208 (Vezy et al., under review). However, this complex entanglement of fine processes is computationally time  
209 and memory consuming, which make the simulations unsuitable for long-term predictions or coarse spatial  
210 scale, especially when working with plantations with high tree densities such as coffee plots (*c.a.* 20 000

211 resprout ha<sup>-1</sup>). One solution to overcome this issue is to build metamodels of MAESPA for some important  
212 outputs of this model.

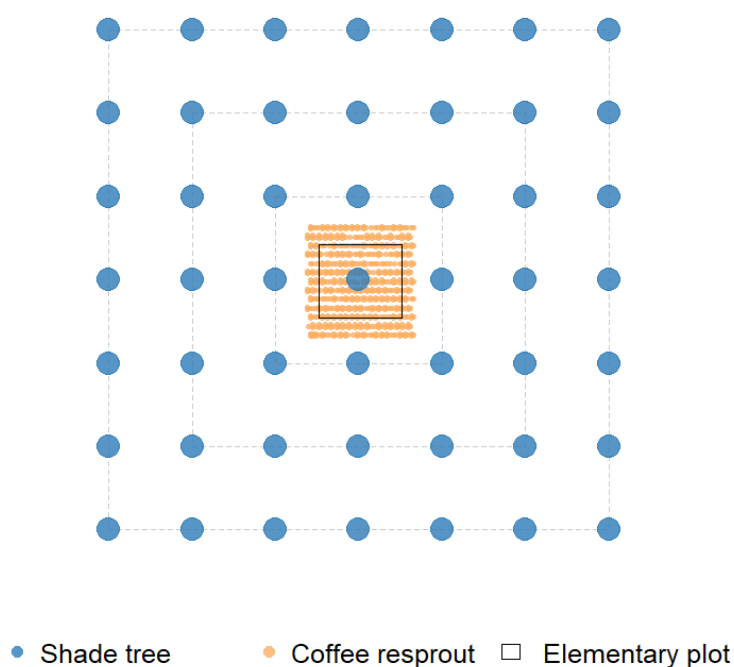
213 Metamodels are made and used to replace complex and time-consuming process-based models by a simple  
214 empirical equation that summarizes and emulates its behavior from the same input data. Therefore,  
215 metamodels are trained to predict an output from the complex model using the maximum range of possible  
216 input conditions to encompass the different processes response at stake within the model. These models are  
217 used for many purposes such as optimization (Razavi et al., 2012; Barton and Meckesheimer, 2006), to extend  
218 the application domain of a model (Sparks et al., 2011), to emulate ensembles of models (Makowski et al.,  
219 2015), to assess the model sensitivity and uncertainty (Christina et al., 2016), or to simply make the model  
220 faster to execute while keeping low error (Marie et al., 2014). Recently, metamodels from MAESPA were  
221 used to develop a plot scale dynamic crop model able to account for the complex heterogeneous canopy  
222 effects on light absorption, light use efficiency, canopy temperature, transpiration, and evaporation of a *Coffea*  
223 *arabica* agroforestry system in Aquiares, Costa Rica (Vezy et al., under review). These metamodels were  
224 trained on a yearly simulation of the plot, and made consistent predictions even outside of the training  
225 conditions (*i.e.* young stages, different shade tree management...). However, it is recommended to train  
226 metamodels on every possible condition on which they will be used to avoid errors coming from either  
227 overfitting or untested process interactions.

228 Therefore, MAESPA was run on all combination of locations (*i.e.* Aquiares and Tarrazu), RCPs (*i.e.* 4.5 and  
229 8.5), shade management (*i.e.* Full Sun, Cordia and Erythrina) and tree density (Table 8) for one randomly  
230 sampled day per month of the 5<sup>th</sup>, 15<sup>th</sup>, 25<sup>th</sup>, 35<sup>th</sup> and 40<sup>th</sup> years after planting, resulting on a set of 2352  
231 simulations. Each simulation was made on two consecutive days to make energy and water balance more  
232 independent from initialization. The coffee was simulated at the shoot level to catch the within-plant leaf area  
233 and crown volume heterogeneity.

234 **Table 8. Simulated scenarios for metamodel training.**

Climate	Location	Shade species and shade tree density (tree ha <sup>-1</sup> )
RCP 4.5	Aquiares	Full Sun: 0
	X	X <i>Erythrina poeppigiana</i> : 200; 250; 350; 400
RCP 8.5	Tarrazu	<i>Cordia alliodora</i> : 50; 75; 100; 125

235  
236 MAESPA was entirely parameterized following Vezy et al. (under review) for both locations. Shade tree  
237 allometric relationships were used to compute their structure according to the species, age and density (Table  
238 9). Each simulated plot was reduced to the minimum representative spatial area by taking its elementary plot  
239 as a Voronoï cell (Figure 23) to optimize computation time. The plot area changed according to the shade tree  
240 density to ensure that 49 shade trees are included in the scene. The coffee trees density remained constant (1.5  
241 coffees.m<sup>-2</sup>) under the different scenarios, therefore the number of coffee plants changed proportionally to the  
242 plot area.



243

244 **Figure 23. Simplified representation of the plot design for MAESPA simulations. Plants outside the elementary plot are used**  
 245 **for light interception computation only, and are present for edge effects.**

246 All MAESPA output variables that are potentially highly impacted by the canopy heterogeneity or the shade  
 247 trees were metamodeled: the direct and diffuse light extinction coefficients of the shade trees which are  
 248 probably the most important factors, the light use efficiency, transpiration, and sensible heat flux from shade  
 249 trees and coffee, the coffee canopy temperature, and its leaf water potential. A constant diffuse and direct light  
 250 interception of the coffee layer was also computed from the MAESPA simulations. Following Vezy et al. (in  
 251 prep.), the metamodels equations were kept as simple as possible, limiting variable transformations, and using  
 252 linear regression only. Any input from MAESPA can be used as explanatory variable for a metamodel,  
 253 ranging from plot-scale structural data (*i.e.* leaf area, leaf area density, shade tree density, average crown  
 254 radius or height, trunk diameter...) to meteorological conditions such as air temperature, vapor pressure,  
 255 photosynthetically active radiation, fraction of diffuse or direct light, wind, air pressure, and atmospheric  
 256 carbon dioxide concentration.

## 257 **2.4. Dynamic crop model**

258 The dynamic crop model used in this study is a plot scale process-based model that was already calibrated and  
 259 validated on Aquiares site (Vezy et al., in prep.). This model was made to simulate coffee plantations under  
 260 any shade management and tree species to uncover their potential effect on light interception, photosynthesis,  
 261 net primary production, number of nodes on plagiotropic branches per surface area that potentially support  
 262 flower buds, number of flowers per surface area, yield, and fruit maturity. Each canopy layer is assumed  
 263 horizontally homogeneous, but spatial-dependent variables are computed using MAESPA metamodels.

264 Carbon allocation is made using a hierarchical allocation scheme with equal priority order to wood from  
265 shoots, coarse roots, and stump, then to fruits which can take all the remaining carbon if needed, and then the  
266 last remaining carbon to leaves and fine roots. The model uses the model from Rodríguez et al. (2011) adapted  
267 at plant level to compute the cohorts of buds and fruits, the positive sensitivity of vegetative growth and  
268 negative sensitivity of inflorescences (*i.e.* number of flowers per inflorescence) to temperature from Drinnan  
269 and Menzel (1995), and the model of Pezzopane et al. (2012) for the bean maturation. The soil and water  
270 balance module are partly derived from the BILJOU model (Granier et al., 2012), and partly from metamodels  
271 for the variables potentially impacted by the canopy heterogeneity (transpiration, sensible fluxes). The model  
272 is entirely parameterized following Vezy et al. (in prep.) excepted for the metamodel equations and  
273 parameters, and the inclusion of the *Cordia alliodora* shade tree species from which the growth is derived  
274 from the equations in Table 9.

### 275 **3. Results**

#### 276 **3.1. Climate projections**

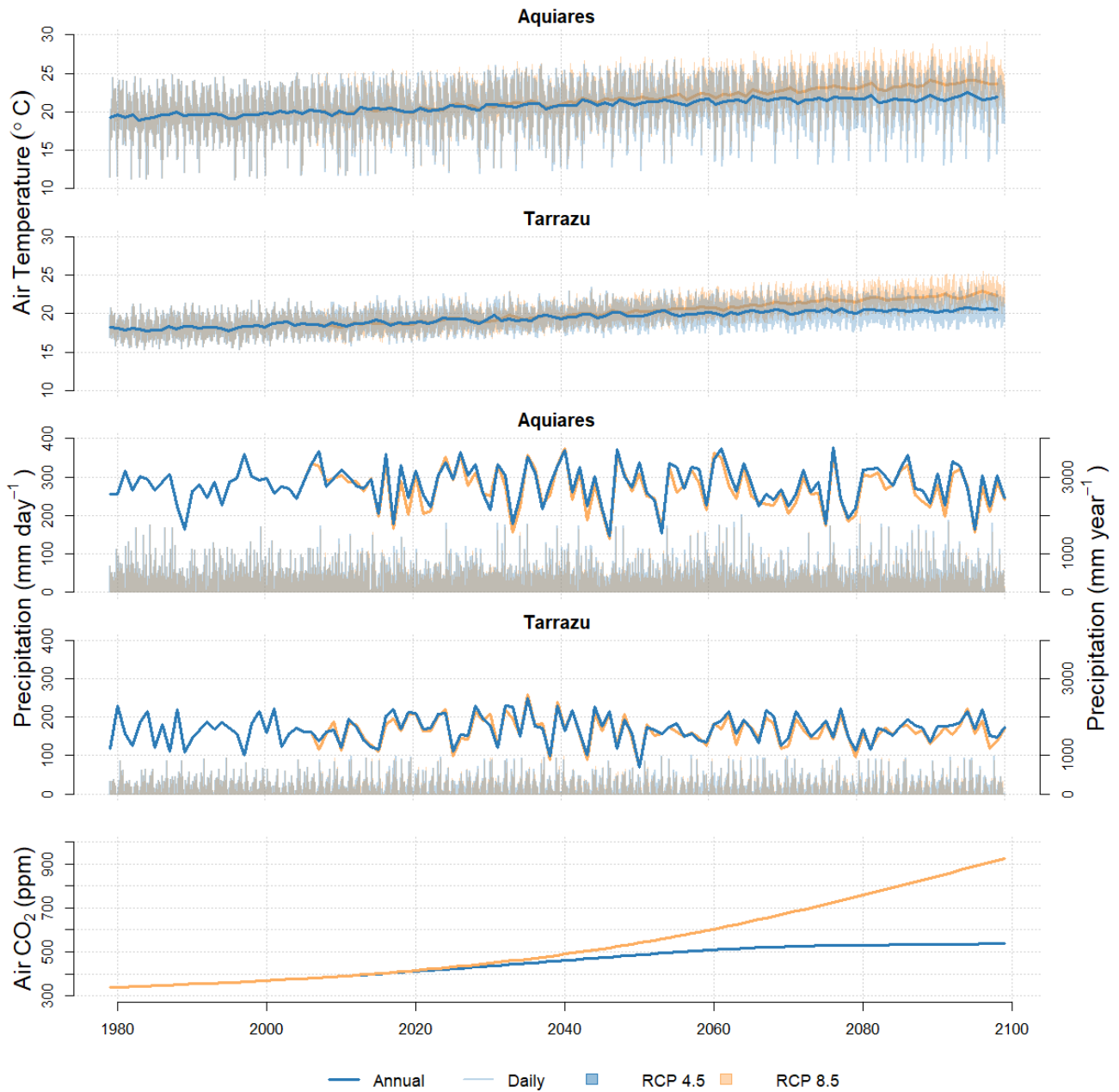
277 The mean annual air temperature (Figure 24) in Aquiares is projected to increase by 0.023°C and 0.041°C per  
278 year in average for RCP4.5 and 8.5 respectively, reaching 21.9°C (+2.6°C compared to 1979) and 23.6°C  
279 (+4.3°C) in 2099. In Tarrazu, the mean annual air temperature is expected to increase from 18.2°C in 1979 to  
280 20.6°C (+2.4°C) and 22.3°C (+4.1°C) in 2099 for RCP4.5 and 8.5 respectively, with a similar average mean  
281 annual increment than for Aquiares site, of +0.024°C and 0.041°C respectively. Tarrazu presented a lower  
282 day-to-day variation of temperature than Aquiares, with an average standard deviation of 0.89°C, half the one  
283 from Aquiares (1.79°C) for both RCPs. Although RCP4.5 presented slightly higher yearly precipitations than  
284 RCP8.5, climate change did not impact much precipitations on the projections, but both sites had very  
285 different regimes. Indeed, annual precipitations in Tarrazu are very variable and rather low (pronounced dry  
286 season), ranging from 688 mm year<sup>-1</sup> to 2599 mm year<sup>-1</sup>, with an average of 1695 mm year<sup>-1</sup> for RCP4.5 and  
287 1647 mm year<sup>-1</sup> for RCP8.5. In Aquiares the range was from 1392 to 3761 mm year<sup>-1</sup>, with an average of 2805  
288 mm year<sup>-1</sup> and 2705 mm year<sup>-1</sup> for RCP4.5 and 8.5 respectively, and hardly any dry season. Hence Tarrazu  
289 experienced c.a. 1100 mm year<sup>-1</sup> less than Aquiares in average. Furthermore, Tarrazu site presented more days  
290 without rain (165 in average) than Aquiares (95 in average), and longer consecutive days without rain, with 41  
291 consecutive dry days in the dry period in average compared to 27 in Aquiares.

292 Atmospheric CO<sub>2</sub> concentrations grew from 337 ppm in 1979 to 538 ppm in 2099 for RCP4.5, and to 927  
293 ppm for RCP8.5. The concentrations reached a plateau under RCP4.5, but not in RCP8.5, which presented a  
294 high growth rate until 2099.



295 Table 9. Allometric equations used to compute plant structure for MAESPA inputs.

Variable	Description	Units	Species	Equation/Value	Source
Htot	Total height		<i>Cordia alliodora</i>	$63.99322 \cdot e^{-1.744 \cdot \text{Age}^{-0.25}}$	Alder and Montenegro (1999)
Hcrown	Crown height		<i>Cordia alliodora</i>	0.35*Total Height	This study
			<i>Erythrina poeppigiana</i>	Trunk height $\times$ %Crown Volume <sup>1/3</sup>	
Rad	Crown radius	meter	<i>Cordia alliodora</i>	$(1.01 + (24.21 * \text{DBH}))/2$	Bullock (2000)
			<i>Erythrina poeppigiana</i>	Crown Height/1.35 $\times$ %Crown Volume <sup>1/3</sup>	This study
D	Trunk diameter		<i>Cordia alliodora</i>	$10^{(\log_{10}(\text{StemDryMass}_{\text{ha}} \cdot \frac{1000}{\text{Tree Density}}) + 0.942)/2.062} / 10$	Segura et al. (2006)
			<i>Erythrina poeppigiana</i>	$0.9/1 + e^{-0.2 \cdot (\text{Age} - 10)}$	This study
Htrunk	Trunk Height		<i>Cordia alliodora</i>	Total height – Crown Height	-
			<i>Erythrina poeppigiana</i>	Max Trunk Height $\times$ $(1 - e^{-0.2 \cdot \text{Age}})$ with Max Trunk Height $\sim U\{3, 4\}$	This study
Vstand	Stand volume	$m^3 \cdot ha^{-1}$	<i>Cordia alliodora</i>	$0.01187 * (\text{Total Height} - 13.5)^{1.961} \times \text{Tree Density}^{0.7527}$	
Wstem	Stem dry mass	$t \cdot ha^{-1}$	<i>Cordia alliodora</i>	$(\text{Stand Volume} \times \text{Wood density})/1000$	Alder and Montenegro (1999)
w	Wood density	$kg_{DM} \cdot m^{-3}$	<i>Cordia alliodora</i>	563	
LA	Leaf Area	$m^2 \cdot tree^{-1}$	<i>Cordia alliodora</i>	FoliageDryMass * SLA	-
			<i>Erythrina poeppigiana</i>	Crown radius <sup>2</sup> $\times$ (Crown Height/2) $\times \pi \times 4/3 \times \text{LAD} \times \%CV$	
SLA	Specific Leaf Area	$m^2 \cdot kg_{DM}$	<i>Cordia alliodora</i>	14.8	Haggar and Ewel (1995)
Wleaf	Foliage dry mass	$kg_{DM} \cdot tree^{-1}$	<i>Cordia alliodora</i>	$-2 + 0.8 \times \text{DBH} \times 100$ Ou $10^{-1.557 + 2.098 \times \log_{10}(\text{DBH} \times 100)}$	Adapted from: Segura et al. (2006)
LAD	Leaf Area Density	$m^2 \cdot m^{-3}$	<i>Erythrina poeppigiana</i>	0.429	Computed from Charbonnier et al. (2013)
PV	Percentage of volume after pruning	%	<i>Erythrina poeppigiana</i>	Spline	Fitted from field expert a priori
				Stump: 0.4224 & 4.22	



296

297 **Figure 24. Annual and daily projected air temperature, precipitation, and atmospheric CO<sub>2</sub> concentrations from downscaled**  
 298 **GCMs for Aquiares and Tarrazu, Costa Rica. See section 2 for more details on the computation.**

299

300 **3.2. Metamodels**

301 The MAESPA metamodels gave good predictions of MAESPA outputs in average (  
 302 Table 10). The light use efficiency (LUE) was positively affected by atmospheric CO<sub>2</sub> concentrations for all  
 303 three plants species, and negatively by the incident PAR reaching the considered layer. The constant coffee  
 304  $K_{Diffuse}$  and  $K_{Direct}$  were found to be equal to 0.40 and 0.35 respectively.

305  
 306 **Table 10. MAESPA metamodel equations and goodness of fit. With  $LUE$  the light use efficiency ( $g_C MJ$ ),  $T_{air}$  (°C) and  $VPD$   
 307 ( $hPa$ ) the air temperature and vapor pressure deficit measured above canopy (and above shade trees if any),  $T_{can}$  (°C) the  
 308 coffee canopy temperature,  $LAI$  the leaf area index ( $m^2_{leaf} m^{-2}_{soil}$ ),  $F_{BEAM}$  (%) the beam fraction of the light and  $PAR_{Above}$   
 309 ( $MJ m^{-2} day^{-1}$ ) the photosynthetically active radiation reaching the layer,  $\Psi$  ( $MPa$ ) the water potential,  $Tr$  ( $mm$ ) the  
 310 transpiration,  $H$  ( $MJ m^{-2}$ ),  $K$  the light extinction coefficient,  $LAD$  ( $m^2_{leaf} m^{-3}_{crown}$ ) the leaf area density,  $Stocking_{Tree}$   
 311 ( $tree m^{-2}$ ) the shade tree density,  $[CO_2]$  the atmospheric carbon dioxide concentration and  $Rad$  ( $m$ ) the average crown  
 312 radius.**

Metamodel	RMSE	R <sup>2</sup>
<i>Coffea arabica</i>		
$LUE = 1.96862 - 0.1286 \cdot PAR_{Abv} - 1.14 \cdot FBEAM + 0.001167 \cdot [CO_2] - 0.012697 \cdot T_{can} + 0.008767$ $\cdot VPD - 1.798841 \cdot \sqrt{F_{BEAM}} - 0.268586 \cdot \sqrt{PAR_{Abv}}$	0.13	0.92
$T_{can} = 0.92921 + 0.95568 \cdot T_{air} + 0.01241 \cdot VPD - 0.47802 \cdot FBEAM + 0.10599 \cdot PAR_{Abv} - 0.04573$ $\cdot LAI_{Tree}$	0.20	0.99
$\Psi_{leaf} = 0.040730 - 0.005074 \cdot VPD - 0.037518 \cdot PAR_{Abv} + 2.676284 \cdot \Psi_{soil}$	0.04	0.87
$Tr_{Coffee} = -0.42164 + 0.03467 \cdot VPD + 0.10559 \cdot LAI_{Cof} + 0.11510 \cdot PAR_{Abv}$	0.13	0.85
$H_{Coffee} = -1.80160 + 0.04265 \cdot T_{air} - 0.06679 \cdot VPD + 2.01274 \cdot FBEAM + 0.25868 \cdot LAI_{Cof}$ $+ 0.58528 \cdot PAR_{Abv}$	0.53	0.88
<i>Cordia alliodora</i>		
$K_{Diffuse} = 0.6218 - 0.1339 \cdot LAD - 21.3615 \cdot Stocking_{Tree}$	0.04	0.80
$K_{Direct} = 0.5913 - 0.1784 \cdot LAD - 18.94 \cdot Stocking_{Tree}$	0.05	0.79
$LUE = 3.219368 - 0.803432 \cdot \sqrt{PAR_{Abv}} - 0.055131 \cdot LAI + 0.001444 \cdot [CO_2]$	0.12	0.95
$Tr_{Tree} = 0.495 + 0.2297 \cdot VPD - 0.0566 \cdot T_{air} + 0.3869 \cdot APAR - 1.2291 \cdot FBEAM - 0.042 \cdot LAI$	0.30	0.93
$H_{Tree} = -1.958 + 0.473 \cdot APAR - 0.2669 \cdot LAI + 6.826 \cdot FBEAM - 0.3481 \cdot VPD + 0.1401 \cdot T_{air}$	0.58	0.67
<i>Erythrina poeppigiana</i>		
$K_{Diffuse} = 0.8861 + 0.09814 \cdot LAI_{Tree} - 0.17232 \cdot LAD_{Tree} - 0.06887 \cdot Rad_{Tree}$	0.006	0.96
$K_{Direct} = 0.75528 + 0.14994 \cdot LAI_{Tree} - 0.18897 \cdot LAD_{Tree} - 0.06135 \cdot Rad_{Tree}$	0.02	0.57
$LUE = 1.612703 - 0.670994 \cdot \sqrt{PAR_{Abv}} + 0.533792 \cdot LAI_{Tree} + 0.001394 \cdot [CO_2]$	0.12	0.94
$Tr_{Tree} = 0.002431 \cdot VPD + 0.256655 \cdot APAR$	0.06	0.96
$H_{Tree} = -0.044597 + 0.850861 \cdot APAR_{Dir} + 0.582084 \cdot APAR_{Dif} - 0.298670 \cdot LAI - 0.02075 \cdot VPD$ $+ 0.007647 \cdot T_{air}$	0.08	0.98

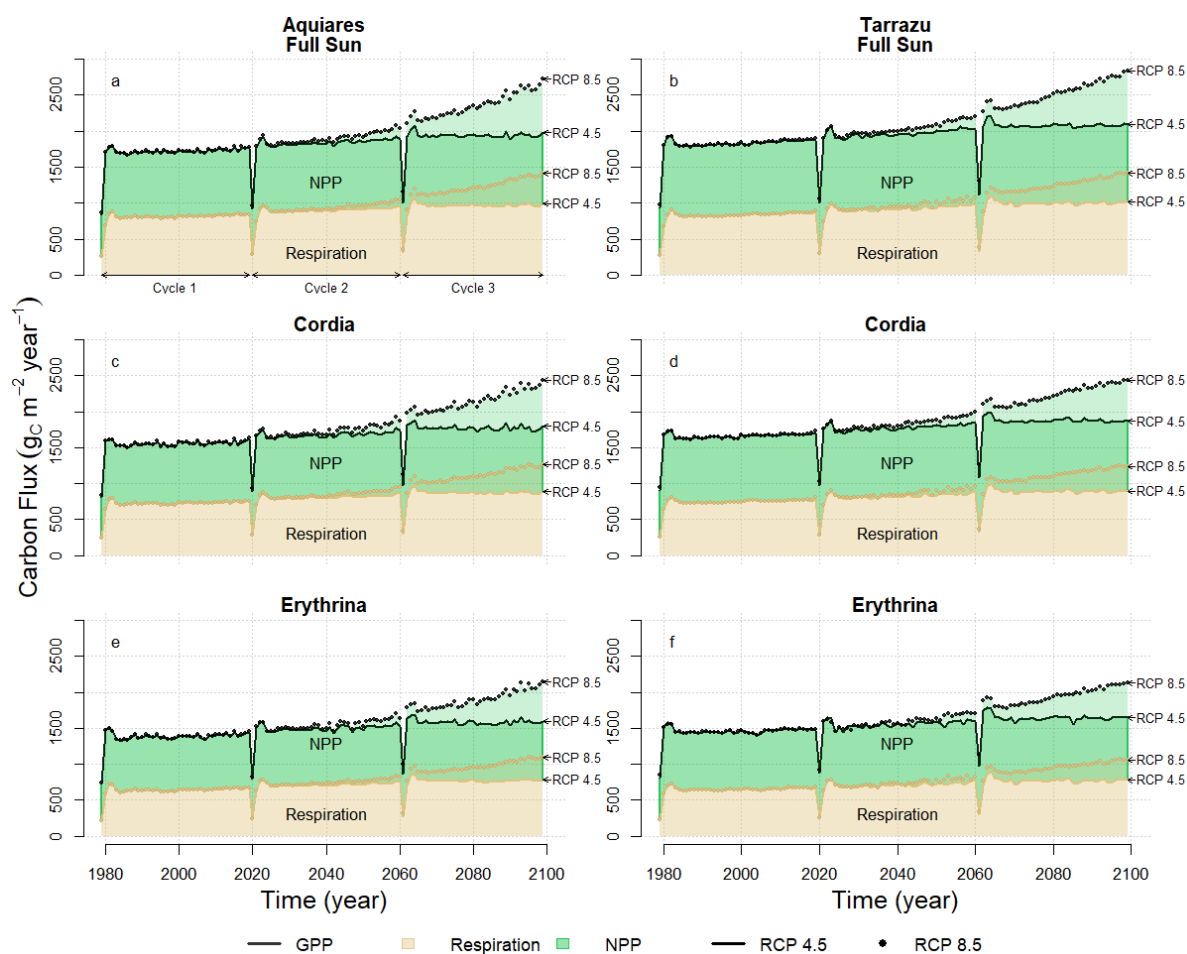
313

### 314 3.3. Climate changes impacts on current coffee plantations

315 Under current conditions in Aquiares during the first planting cycle (i.e. 1979 to 2020), coffee NPP was  
316 higher under Full Sun management compared to Cordia (-8.6%) or Erythrina management (-17.7%). This was  
317 due to a coupled effect of a reduced increased primary production (GPP) in Full Sun, and higher respiration on  
318 the overall cycle (Figure 25). However, although the coffee absorbed PAR was reduced by 21.8% under  
319 Cordia management and by 34.7% under Erythrina, the compensation effect due to increased LUE (+14.4%  
320 and +25.3% resp.) gave only a 9.5% and 19.2% reduction of GPP. The shade management effect had the same  
321 impact in Tarrazu, but with different absolute NPP values: Full Sun NPP in Tarrazu was 8.6% higher than in  
322 Aquiares, and Cordia and Erythrina management gave 9.1% and 9.6% higher NPP than in Aquiares with the  
323 same treatments. This was mainly due to higher incoming PAR in average per year in Tarrazu. GPP,  
324 respiration, and NPP increased under climate change whatever the RCP for all managements and both  
325 locations. Under high CO<sub>2</sub>, GPP increased rather exponentially due to photosynthesis enhancement. This  
326 phenomenon was correlated to the different trends in atmospheric CO<sub>2</sub> concentrations between the two RCPs  
327 (Figure 24). But autotrophic respiration similarly. Therefore, GPP increased linearly between each growing  
328 cycle under RCP4.5 projections, and its trend became exponential under RCP8.5. NPP increased also, but  
329 only marginally whatever the scenario. The difference between the two RCPs started impacting increasingly  
330 GPP and respiration from *c.a.* 2040.

331 In coffee, vegetative growth relies on nodes (which can also bear inflorescences) and internodes. The  
332 simulated vegetative growth increased under higher temperatures (Figure 26): the number of nodes per coffee  
333 increased with climate change, especially in Aquiares under RCP8.5, with an average increase of 1.26 nodes  
334 year<sup>-1</sup>, compared to 0.58 nodes year<sup>-1</sup> under RCP4.5. Tarrazu number of nodes increased more slowly, with  
335 only 0.09 nodes year<sup>-1</sup> under RCP4.5 and 0.34 nodes year<sup>-1</sup> for RCP8.5. The number of flowers decreased  
336 progressively with increasing air temperature in Aquiares, leading to less flowers in average under RCP8.5.  
337 The number of flowers in Tarrazu increased in average for both RCPs during the second growing cycle but  
338 became more variable at the same time, and variability continued to increase in the third cycle for RCP4.5.  
339 Values severely dropped under RCP8.5, while decreasing in variability. It appeared that the high variability  
340 was mainly correlated to the bud initiation period that started increasingly earlier under high seasonal  
341 temperature, reducing the bud dormancy during the dry period, and then becoming highly dependent on the  
342 precipitations during this period to provoke bud break. A second consequence is that the more the dry period  
343 is pronounced, the more synchronized is the blossoming, which results in less aborted buds, and therefore  
344 more flowers. Agroforestry allowed a slightly higher number of flowers under high temperature, with  
345 approximately 9.7% more flowers during the third cycle under RCP8.5 in Aquiares for Cordia and 8.3% for  
346 Erythrina management, and 4.8% and 6.9% more in Tarrazu under Cordia and Erythrina as compared to Full  
347 sun. However, like in Full Sun, the number of nodes was reduced by 1.8% (1.4%) and 3.4% (3.7%) under  
348 RCP8.5 (RCP4.5 resp.) for Cordia and Erythrina management respectively in Aquiares, and by 1.5% (1.7%)  
349 under RCP8.5 (RCP4.5 resp.) for Cordia in Tarrazu. There was no significant difference in the number of

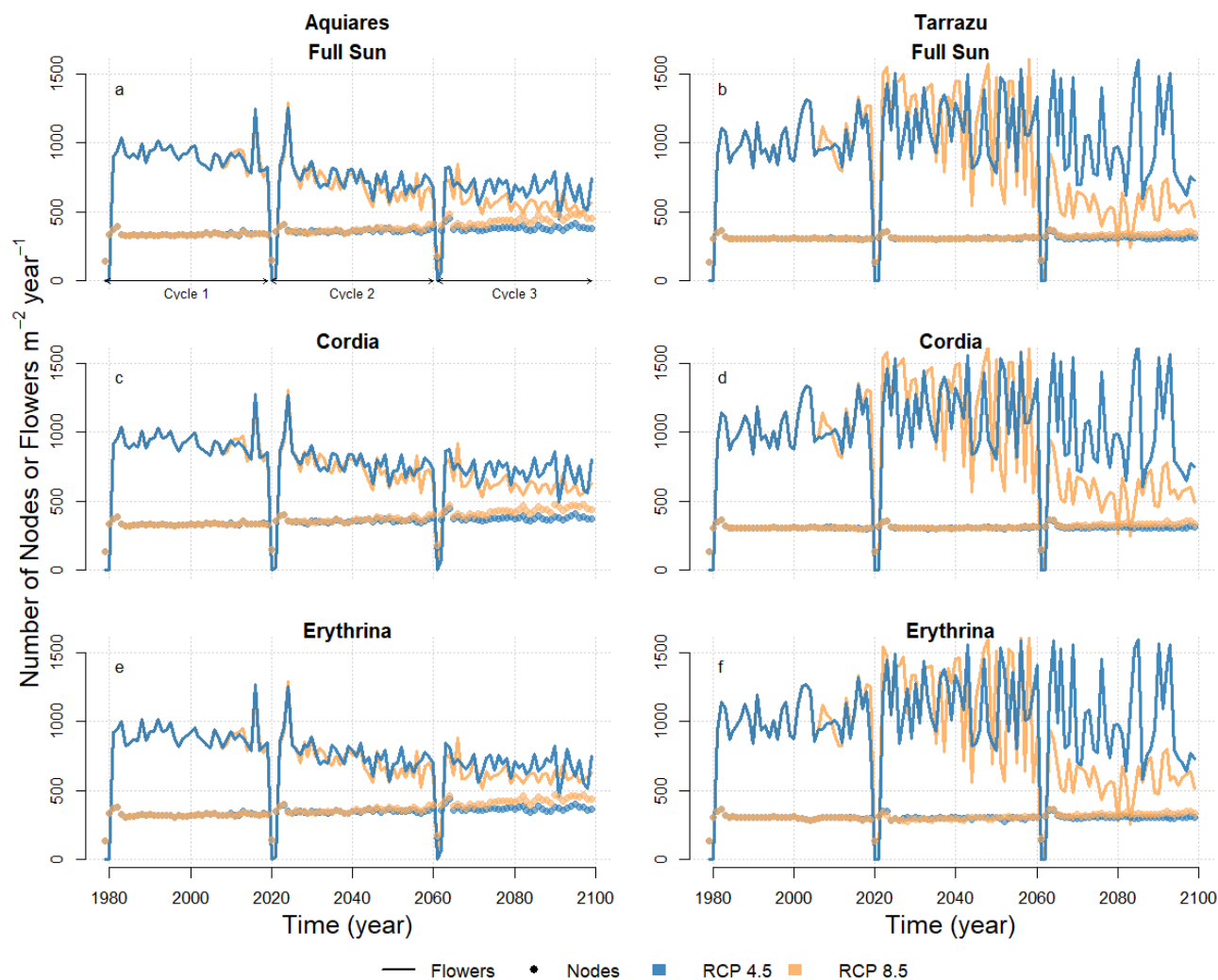
350 nodes between Full Sun and Erythrina management in Tarrazu, because the period of the coffee vegetative  
 351 development corresponds to the period of lowest shade trees LAI.



352  
 353 **Figure 25. Climate change impacts on GPP and cumulated respiration and NPP according to Representative Concentration**  
 354 **Pathways (RCP 4.5 and RCP 8.5); location (left: Aquiares, right: Tarrazu) and current reference management: coffee grown**  
 355 **in monoculture (a,b) or in agroforestry systems under *Cordia alliodora* (c,d) or *Erythrina poeppigiana* (e,f).**

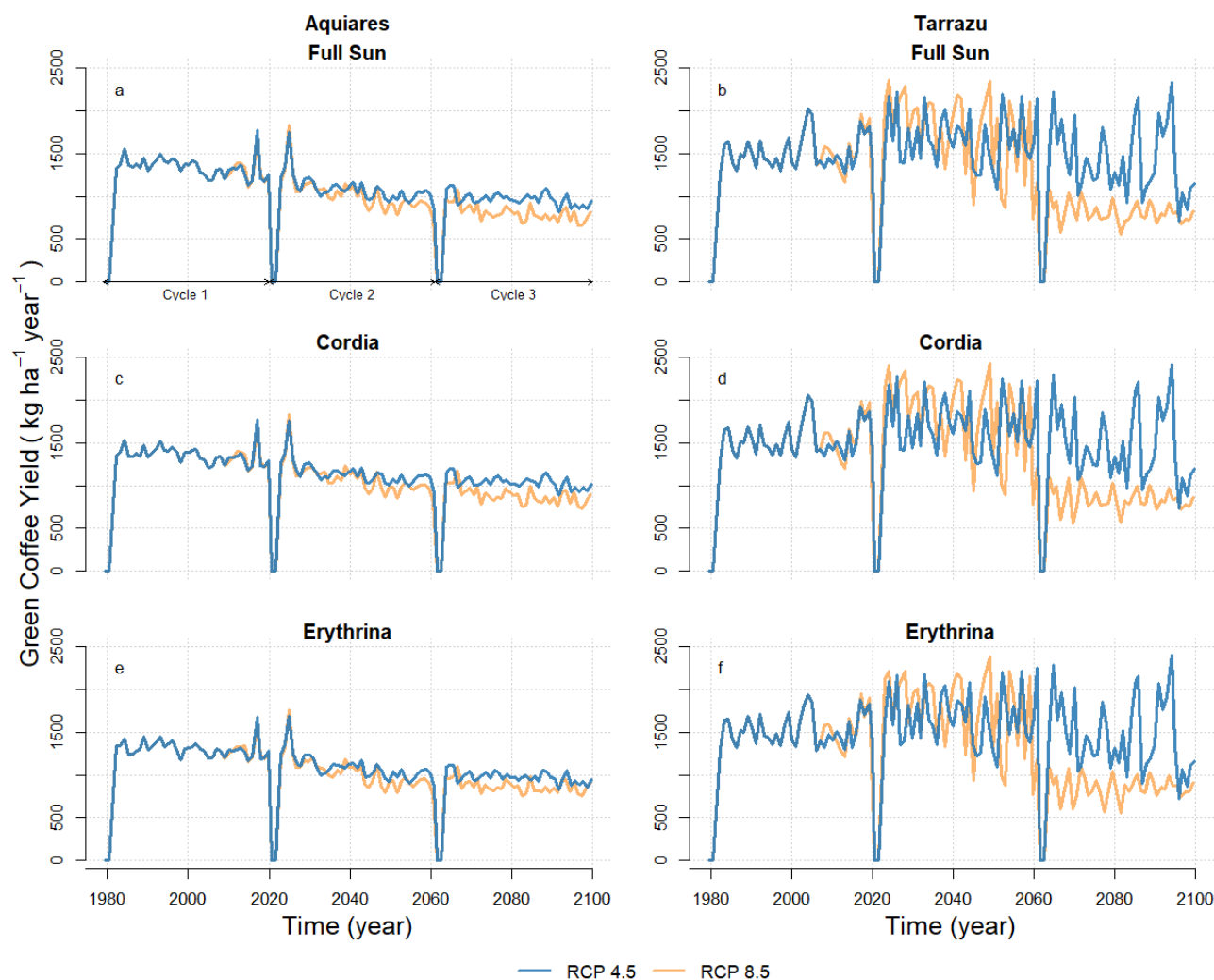
356 The green coffee yield was closely related to the number of flowers per coffee plant. Hence, coffee bean  
 357 production in Aquiares was negatively impacted by climate change (Figure 27), especially for RCP8.5,  
 358 coming from a cumulated 49.8 tons of green coffee per hectare during the first cycle, to 36.0 t ha<sup>-1</sup> cycle<sup>-1</sup> (-  
 359 27.9%) on the third cycle under Full Sun management. Management with *Cordia* shade trees slightly  
 360 increased green coffee yield in the first cycle (+1.2%), and this effect became increasingly positive with time,  
 361 with +5.0% and +6.0% for RCP4.5 and 8.5 respectively for the second cycle, and coming up to 7.1% and  
 362 9.6% for the third cycle compared to Full Sun at the same period. Erythrina management gave lower yield  
 363 under current conditions (-2.8%, cycle 1), same yield on the second cycle, and increased yield on the third  
 364 cycle compared to Full Sun at the same period, with +3.7% under RCP4.5, and +7.9% under RCP8.5. The  
 365 same effects were simulated in Tarrazu, with a positive effect of *Cordia* management starting on Cycle 1, and  
 366 increasing over time until +2.9% and +7.1% under RCP4.5 and RCP8.5 respectively in the third cycle, and no  
 367 effect for Erythrina in the second cycle, but an increased yield for cycle 1 (c.a. +1.1% for both RCPs) and  
 368 cycle 3 (+2.3 and +1.1% for RCP4.5 and 8.5 resp.) compared to Full Sun. However, it should be noted that

369 bean production increased from the first to the second cycle for both RCPs, but collapsed to half the values of  
 370 the first cycle in the third one under RCP8.5. Although the decrease remained by only 2% under RCP4.5, the  
 371 variability between years became huge. The overall coffee bean maturity at harvest decreased with increasing  
 372 temperature in both locations (data not shown). This effect comes from the shorter time fruit had to  
 373 accumulate sugar before maturity, because harvest was performed sooner than in current conditions, a  
 374 consequence of higher maturation speed. The difference between RCP4.5 and RCP8.5 was marked more in  
 375 Tarrazu than in Aquiares. No difference was found between shade management for bean maturity.



376  
 377 **Figure 26. Climate change impacts on the number of nodes (vegetative growth + sites for inflorescences) and flowers per coffee**  
 378 **plant according to representative concentration pathways (4.5 and 8.5); location (left: Aquiares, right: Tarrazu) and current**  
 379 **reference management: coffee grown in monoculture (a,b) or in agroforestry systems under *Cordia alliodora* (c,d) or *Erythrina***  
 380 ***poeppigiana* (e,f).**

381



382

383 **Figure 27.** Climate change impacts on coffee yield according to representative concentration pathways (4.5 and 8.5); location  
 384 (left: Aquiares, right: Tarrazu) and current reference management: coffee grown in monoculture (a,b) or in agroforestry  
 385 systems under *Cordia alliodora* (c,d) or *Erythrina poeppigiana* (e,f).

### 386 3.4. Disentangling CO<sub>2</sub> and temperature effects

387 Increased [CO<sub>2</sub>] and air temperature are expected to have opposite effects on coffee GPP through their  
 388 influence on LUE (

389 Table 10), but NPP was slightly increased under both locations and both RCPs, pointing out that [CO<sub>2</sub>] effect  
 390 was more than compensating the temperature effects (Figure 27). A simulation experiment confirmed this  
 391 result: NPP of Full Sun coffee grown with the projected [CO<sub>2</sub>] increase, but no air temperature increase raised  
 392 by +43.1% (comparison of the last ten years of the first and third cycles). Conversely, NPP of Full Sun coffee  
 393 grown with the projected increase air temperature but no increase in [CO<sub>2</sub>] decreased by 11.2% in the last ten  
 394 years of the third cycle compared to the last ten years of the first cycle. When both [CO<sub>2</sub>] and air temperature  
 395 were rising, NPP increased by +25.5%. This confirmed that the positive [CO<sub>2</sub>] effect on NPP was largely  
 396 compensating the negative air temperature effect (Figure 28).

397 Fruit production remained approximately constant between cycles when increasing [CO<sub>2</sub>] only. This  
 398 phenomenon shows that fruit production was not limited by carbon offer in the model, because fruit  
 399 production did not increase with increasing NPP (Table 11). However, increased air temperature had negative  
 400 effect throughout the entire simulation in Aquiares. For Tarrazu, the result is different: the increase in  
 401 temperature had a positive effect during the first and second cycle, but the effect became negative in the third  
 402 cycle. These processes are the result of the double dependence of fruit on air temperature. First, NPP offer was  
 403 always high enough to never limit the fruit carbon demand, because this compartment has one of the highest  
 404 priority of resource allocation (*i.e.* up to 90% of the offer), even in the simulation where air temperature was  
 405 increased but [CO<sub>2</sub>] remained constant. Second, the bud initiation process is positively linked to air  
 406 temperature until the mean diurnal temperature reaches a threshold of 23°C, after which the link becomes  
 407 negative. Therefore, the fruit production and final yield increases until reaching an optimum with air  
 408 temperatures around 23°C, and then decrease because the number of flowers decreased.

409 **Table 11. Key variables of coffee simulations for the third cycle average (2060-2099) compared to the reference +CO<sub>2</sub>/+T° of**  
 410 **the first cycle (1979-2019) for RCP8.5 in Aquiares.**

Projection	T°	CO <sub>2</sub>	NPP	GPP	LUE	Respiration	Flowers	LAI	Yield
+CO <sub>2</sub> /+T°	+3.37°C	+107%	+25.5%	+37.0%	+34.2%	+50.0%	-36.8%	=	-40.0%
-CO <sub>2</sub> /+T°	+3.37°C	-	-11.2%	-4.2%	-4.4%	+3.6%	-36.8%	=	-40.0%
+CO <sub>2</sub> /-T°	-	+107%	+43.1%	+41.0%	+38.7%	+38.8%	=	=	-2.1%

### 411 3.5. How management impacts coffee yield

412 The differences between shade tree managements of both location and both RCP are presented in Figure 29.  
 413 Two scenarios of Cordia management were simulated: thinned whenever the transmittance was lower than 0.7  
 414 (reference) or 0.4 (adapted). Managements with lower transmittance thresholds than 0.4 gave systematically  
 415 lower yield, and transmittance higher or in-between gave results very close to the ones presented. Cordia  
 416 shade tree density decreased progressively during the cycle due to thinning, until reaching 13.1 trees ha<sup>-1</sup> for  
 417 the 0.4 transmittance threshold and 4.3 trees ha<sup>-1</sup> for 0.7 transmittance threshold. Erythrina management  
 418 showed the best compromise between shade and yield with reduction of pruning during coffee bud initiation.  
 419 All other tests on adaptations of management were found to give lower yields than the reference and were not  
 420 presented here. Among all managements, agroforestry was never able to compensate totally the negative  
 421 effect of future increase of air temperature to maintain the current yield, climate being the leading factor for  
 422 coffee bean production. However, although coffee yield under current conditions required low shade, shade  
 423 became increasingly beneficial with future conditions, especially under RCP8.5. Indeed, in both locations and  
 424 both RCPs, Cordia reference management started improving yield under future 2050-2060 conditions for both  
 425 RCPs and locations, and Cordia adapted management gave even higher yield relative to Full Sun in Aquiares  
 426 RCP8.5.



427

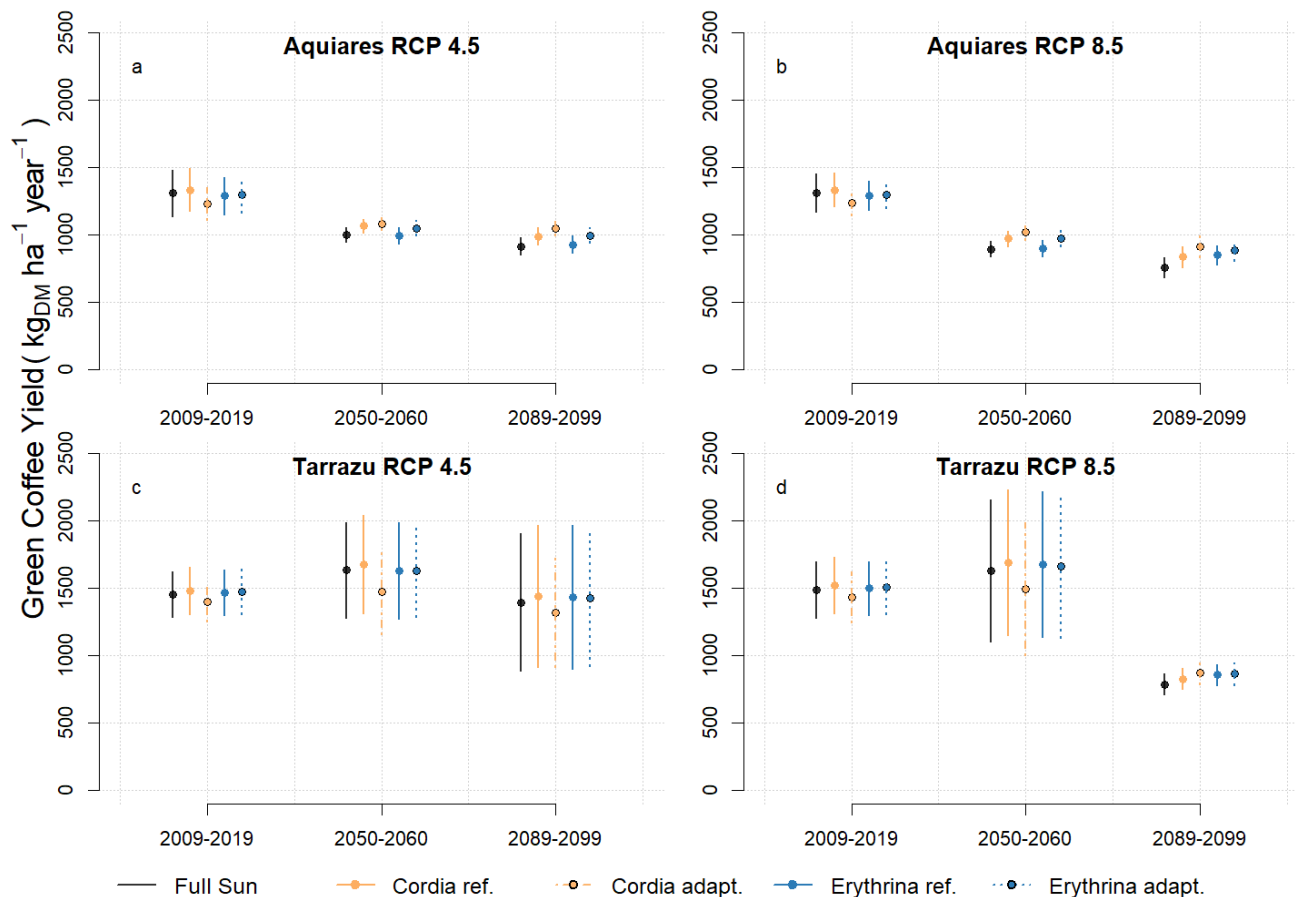


428

429 **Figure 28. CO<sub>2</sub> and air temperature increase effect on coffee NPP and Yield. +CO<sub>2</sub> is a modeling scenario with [CO<sub>2</sub>] increase,**  
 430 **while +T° is a scenario with air temperature increase.**

431 The period 2089-2099 was the hottest conditions experienced by the coffee in the simulations. Under these  
 432 future conditions in Aquiares, Cordia under reference management gave higher yield than Full Sun (+8.1%  
 433 and +10.6% RCP4.5 and 8.5 resp.), and Cordia under adapted management gave the highest yield between all  
 434 managements for both RCPs, with +14.7% under RCP4.5 and even +20.9% under RCP8.5 (Figure 29a-b).  
 435 Furthermore, Cordia adapted management only lost 2.9% of yield between the second and the third cycle in  
 436 Aquiares RCP4.5 (Figure 29a), instead of the 8.6% for Full Sun management, making this management not  
 437 only the best for absolute yield under future conditions, but also the management with the lowest decreasing  
 438 trend with climate change. Erythrina current management (*i.e.* reference) only started to give higher yields  
 439 than full sun in the end of the third cycle (+1.4% and +12.4% for RCP4.5 and 8.5 resp.), but gave higher  
 440 yields when adapted (*i.e.* reduced pruning) starting from the end of the second cycle (+4.8% and +8.9%  
 441 compared to Full Sun), and even higher relative yield at the end of the period (+8.7% and +16.7% for RCP4.5  
 442 and 8.5 resp.). Cordia adapted management between 2089 and 2099 gave higher yield than the Full Sun  
 443 management between 2050 and 2060 for both RCPs in Aquiares (Figure 29a-b). In Tarrazu (Figure 29c-d),  
 444 Cordia reference management was always slightly better than Full Sun (+2.1% to +3.3%). Despite a higher

445 variability in Tarrazu, the Cordia reference management always gave higher yield than any management,  
 446 except at the end of the last cycle under RCP8.5 (Figure 29d), when Cordia adapted management gave the  
 447 highest yield (+10.5% compared to Full Sun), closely followed by the Erythrina adapted management (+9.5%  
 448 compared to Full Sun).



449  
 450 **Figure 29.** Average and standard deviation of the green coffee yield for crop age 29 to 39 (last 10 years of the third cycle),  
 451 representing historic (2009-2019), short-term (2050-2060) and mid-term (2089-2099) coffee production of coffee grown in  
 452 monoculture (Full Sun), under *Cordia alliodora* reference management (current, thinning as soon as the light transmittance is  
 453 under 0.7) or adapted management (thinning as soon as the light transmittance is under 0.4), or under *Erythrina poeppigiana*  
 454 reference management (pruned twice a year, stocking= 200 tree ha<sup>-1</sup>) or adapted management (pruned once a year, stocking=  
 455 200 tree ha<sup>-1</sup>). Historic results differ between RCPs because climate start differing from 2005.

## 456 4. Discussion

### 457 4.1. Model coupling

458 The coupling of the two models through metamodells allowed the plot-scale model to integrate the high infra-  
 459 plot spatial heterogeneity in agroforestry system, even if this is no more explicit in the outputs of the  
 460 metamodells or the crop model (*i.e.* only one value for the coffee layer). This is particularly of interest for  
 461 plantations with low density of shade trees because light transmittance become increasingly anisotropic with  
 462 shading tree inter-distance (Charbonnier et al., 2013). Furthermore, metamodells allowed the dynamic crop  
 463 model to compute complex physiological interactions such as the negative effect of temperature and positive

464 effect of shade and CO<sub>2</sub> fertilisation on light use efficiency, without hard-coding the equations and with low  
465 simulation time. Moreover, using a 3D “complex” model such as MAESPA allows an easier parametrisation  
466 actually: indeed, most of the parametrisation is done at leaf or tree level, the most frequent level for field  
467 measurements. Parameterizing a plot-scale model generally requires an up-scaling procedure which can be  
468 highly uncertain on such heterogeneous canopies. This method was indispensable to assess the effects of new  
469 environmental conditions under climate change, and complex structural managements using thinning or  
470 pruning on coffee yield simulations. For example, it was found in the metamodels that light use efficiency was  
471 higher under shade than in full sun Charbonnier et al. (2017). Note that even if in the final model the coffee  
472 layer is considered homogeneous, its variables (*e.g.* LUE, etc.) represent the average functioning obtained  
473 with MAESPA “heterogeneous” simulations, *i.e.* with coffee canopy under a large range of incoming PAR  
474 depending on the location of the coffee under a continuous shade effect. The approach is therefore totally  
475 different than other models which take shade as a rather simpler factor (*e.g.* shaded or non-shaded), or at best  
476 compute coffee grown under shade tree and in full sun separately, and then average the simulation results with  
477 a shade weight (Van Oijen et al., 2010b). Metamodels also made the model substantially faster because they  
478 summarise many processes into one simple equation and this simple equation can be used elsewhere readily,  
479 without running complex models.

#### 480 **4.2. Climate change impacts on coffee production**

481 Future climate changes influenced many processes that impact coffee net primary production and bean  
482 production. First, the higher CO<sub>2</sub> concentration compensated the negative effect of temperature increase on  
483 photosynthesis in the model. The respiration also increased with higher temperature, but not as fast as GPP,  
484 which led to increased NPP under climate change, especially under RCP8.5. These results are in agreement  
485 with Rodrigues et al. (2016) that found an increase in coffee assimilation under elevated 700 ppm CO<sub>2</sub>  
486 concentrations compared to the reference 380 ppm, even under very high average temperature of 42°C during  
487 the day and 34 °C during the night. These results show that *Coffea arabica* could have a high resilience to  
488 temperature, and hence benefit from climate change, at least for its vegetative development. Furthermore, the  
489 model predicted a higher wood production, higher reserve pool, and higher number of nodes per coffee plant  
490 under climate change, thanks to the higher average temperature during the vegetative development. However,  
491 yield decreased with increasing air temperature in Aquiares due to a higher level of flower abortion, and  
492 increased and then decreased in Tarrazu, while GPP and NPP seemed uncorrelated to yield. Indeed, the carbon  
493 offer was always higher than the fruit carbon demand, making GPP not limiting for fruit growth but yield was  
494 directly affected by air temperature. Drinnan and Menzel (1995) found the same results, with optimum daily  
495 air temperature as high as 30.5°C for vegetative development during summer, but optimum daily air  
496 temperature of 20.5°C for reproductive development, and our model is actually built around their results. Gay  
497 et al. (2006) found through their multiple regression model that seasonal air temperature was also the main  
498 determinant for coffee production. We built our model around the hypothesis that the air temperature effect is

499 not only coming through a link between air temperature and GPP, but also through a direct link of temperature  
500 on the flowering and grain filling process.

501 Fruit maturation was directly linked to the fruit growing duration, because fruit accumulated sugar when  
502 maturing (Pezzopane et al., 2012). Therefore, as fruits grew more rapidly under climate change, their maturity  
503 decreased accordingly.

504 The different elevation between Aquiares and Tarrazu led to distinct results. Aquiares experienced a much  
505 warmer and rainier climate than Tarrazu all along the studied period. Due to higher elevation and lower  
506 temperature, Tarrazu coffee had a longer bud initiation period than Aquiares. In Aquiares, budbreak and  
507 flowering occurred later due to a lower average temperature during bud development. This phenomenon  
508 explained the higher predicted production in Tarrazu under current climate, which was also observed  
509 comparing the yield in Meylan (2012) for Tarrazu with an average of 3.15 t ha<sup>-1</sup> under Erythrina and  
510 Charbonnier et al. (2017) with 2.56 t ha<sup>-1</sup> for Aquiares under Erythrina also. Tarrazu simulated yield presented  
511 more inter-annual variability because the precipitations were more variable than in Aquiares, making the fruit  
512 development variable between years. Such variability was confirmed in Meylan (2012), with 207% variability  
513 in yield in average (up to 317%) between 2010 and 2011, while variability between two years in Aquiares  
514 found in Charbonnier et al. (2017) was 116.5% only. Simulations of the number of flowers and yield in  
515 Tarrazu increased in average in the second cycle, indicating that current air temperature is lower than the  
516 optimum for reproductive development nowadays. Mean annual air temperature in Tarrazu remained lower  
517 than the current one (*i.e.* 2017) in Aquiares almost until the end of the simulated period (*i.e.* 2093) under  
518 RCP4.5 and until 2062 under RCP8.5. Yield variability also increased with climate change, because the coffee  
519 reproductive development was shorter due to increased air temperature, making the bud dormancy break  
520 occurring within the dry period, which further enhance the variability because of the highly scattered  
521 precipitations during this period. These results show that a possible enhancement in yield is expected in high  
522 elevation areas until *c.a.* 2060. Afterward, a decrease in yield is expected in all elevations, especially on sites  
523 with a marked dry period if the climate change follows the RCP8.5 pathway. Schroth et al. (2009) found  
524 similar results using the MAXENT species distribution model, which predicted that coffee suitability will  
525 move to higher elevations under climate change around 2050 also, mainly due to more optimal air  
526 temperature.

### 527 **4.3. Optimizing management for future conditions**

528 Shade management could not compensate for climate change effect in any case scenario, but still could  
529 increase the yield compared to full sun management.

530 Adding shade trees above the coffee layer decreased NPP substantially but increased the yield. However, the  
531 shade effect was not always positive, and a careful attention must be given for shade tree management to  
532 optimize the shade impact on the complex interactions between transmitted light for photosynthesis and air  
533 temperature for flower development. Our results showed that shade management will become increasingly

534 relevant with climate change because it has the potential to improve yield, and compensate for temperature  
535 increase to some extent (*e.g.* yield loss between cycle 2 and 3 was less severe under shade management).  
536 However, the optimal shade management to follow will depend on local climatic conditions and on the pace  
537 of climate change. In any case, in the considered regions of this study, it will probably have to shift towards a  
538 higher shade level (*i.e.* higher shade LAI and lower transmittance) to sustain coffee bean production. These  
539 results are in agreement with Lin (2007), who found that higher shade levels tends to decorrelate the  
540 temperature and the coffee yield, which is precisely what was found in this study because increased shade  
541 reduced the trend of the negative air temperature effect. In Tarrazu, Cordia reference management was also  
542 the best under current conditions, and remained likewise throughout the whole period, excepted under  
543 particularly warm climate of RCP8.5 in the end of the period (2089-2099) under which Cordia adapted  
544 management became better, closely followed by Erythrina adapted management. Furthermore, it has been  
545 shown that nutrient availability would probably constrain productivity under enhanced atmospheric CO<sub>2</sub>  
546 concentrations (Ellsworth et al., 2017). Coffee plantations are generally highly fertilized, and were  
547 consequently not considered to be limited by nutrients in this study, but it could be interesting to include  
548 nutrient limitation effect in the model to foresee what would be their impact on coffee production, especially  
549 if nutrient costs rises in the future (Fixen and Johnston, 2012).

550 Overall, our results show that the current managements could be applied to future conditions with little  
551 adaptation, using less thinning events for Cordia, and less pruning events for Erythrina to increase the shade  
552 level, which requires less labour for thinning or pruning, and hence gives higher profits in the end. But as  
553 shade management will have an increasing effect on yield with climate change, more attention must be given  
554 to optimize the light and temperature trade-off in the future to sustain less temperature and light during bud  
555 initiation, and more light and temperature during vegetative development (Drinnan and Menzel, 1995).  
556 Therefore, even more managements should be tested, such as multi-species shade management to harness the  
557 benefits of different trees species by coupling the high flexibility and nitrogen fertilization of the pruned  
558 Erythrina management and the less labour-demanding Cordia management that increase revenue stability with  
559 wood export. Then, it is possible that stakeholders could sustain coffee production in the future by leveraging  
560 the different solutions to adapt coffee crops to climate change, such as genetic selection and agroforestry.

## 561 **5. Conclusion**

562 Two coffee plantations areas were modelled using a dynamic crop model coupled to the 3D explicit MAESPA  
563 model using metamodels to allow the former to simulate the spatial anisotropic effect induced by shade trees.  
564 Metamodels gave satisfactorily results despite using simple regression equations with few variables. Coffee  
565 net primary production was enhanced in the future by the increase in [CO<sub>2</sub>] that compensated and even  
566 exceeded the negative effect of increased air temperature. However, yield reduced progressively in lowlands  
567 from now, while increased until *c.a.* 2060 and then decreased until 2100 in more elevated plots. Future yield  
568 was linked to the number of flowers produced by the plant, but not ostensibly to the NPP because carbon offer

569 always met fruit carbon demand under elevated [CO<sub>2</sub>]. Our study emphasizes that although growing coffee  
570 under agroforestry was found increasingly beneficial for yield while climate became stressfully warmer, it  
571 only could mitigate a fraction of the losses, so it cannot be thought as the only solution to consider. Most of  
572 the negative effects of climate changes on yield were not compensated, and neither CO<sub>2</sub>, nor shade were  
573 sufficient to avoid large yield losses. Only higher elevation was efficient but for a limited time and limited  
574 space only. We consider that other forms of adaptation must be combined, such as breeding, grafting, and  
575 using vigorous hybrids. Moreover, we stress that to date, there is still no field experiment combining CO<sub>2</sub> and  
576 T° over a range of cultivars to study their effects on the reproductive phenology of coffee: this knowledge gap  
577 severely impede projections and models today.

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#### 4.4. Conclusion du chapitre

Deux plantations de café issues de deux sites différents au Costa Rica ont été modélisées. Pour se faire, un modèle dynamique de culture a été couplé à un modèle 3D, MAESPA, grâce à l'utilisation de métamodèles pour permettre au premier de simuler les effets d'hétérogénéité spatiale induits par les arbres d'ombrage. Les métamodèles ont donné des résultats satisfaisants malgré l'utilisation d'équations de régression simples avec peu de variables. Les simulations montrent que la production primaire nette du café augmente à l'avenir grâce à l'augmentation de la  $[CO_2]$  qui compense et même dépasse l'effet négatif de l'augmentation de la température de l'air. Cependant, le rendement diminue progressivement tout au long de la période jusqu'en 2100 pour le site le moins élevé, et augmente jusqu'à environ 2060, puis diminue jusqu'en 2100 dans la parcelle plus en altitude. Le rendement est fortement lié au nombre de fleurs produites par la plante, mais pas à la NPP en apparence car l'offre de carbone est toujours supérieure à la demande des fruits sous une  $[CO_2]$  élevée. Notre étude montre que bien que la culture du café sous agroforesterie soit de plus en plus bénéfique pour les rendements de café sous climats stressants, elle n'atténue qu'une fraction des pertes, et n'est donc pas la seule solution à prendre en compte. La plupart des effets négatifs des changements climatiques sur le rendement n'ont donc pas été compensés, et ni le  $CO_2$ , ni l'ombrage ne sont suffisants pour éviter les grandes pertes. Ainsi, seule une altitude plus élevée s'est montrée efficace, mais uniquement pour un temps limité. Par conséquent, nous considérons que d'autres formes d'adaptation doivent être combinées, telles que l'utilisation d'hybrides plus résistants aux températures. En outre, nous soulignons qu'à ce jour il n'existe toujours aucune expérimentation combinant  $CO_2$  et  $T^\circ$  sur une gamme de différents cultivars pour étudier ces effets sur la phénologie du café, ce qui entrave sérieusement le paramétrage et la validation des modèles, et donc les projections.



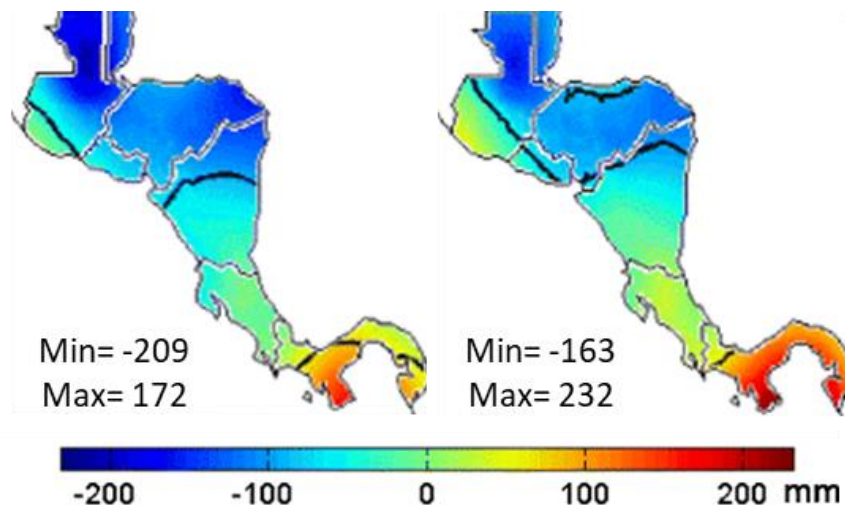
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## 5.1. Simulation des changements climatiques

Les changements climatiques simulés pour les deux sites au Costa Rica ont montré une augmentation de la température moyenne de 2.2°C pour le RCP4.5 et *c.a.* 4.1°C pour RCP8.5 entre la période historique (1986-2005) et la période 2089-2099. Cette augmentation se situe dans les valeurs hautes comparativement à l'augmentation de la température à l'échelle globale simulée en moyenne par les GCM, qui est de 1.8°C (intervalle de confiance 5-95% : 1.1°C et 2.6°C) sous RCP4.5, et 3.7°C (2.6 à 4.8°C) sous RCP8.5 (Pachauri et al., 2014). Cependant, les deux sites ne montraient aucun changement significatif de leur régime de pluie dans le futur, que ce soit en quantité ou en fréquences. Cet effet peut s'expliquer par la position particulière des deux localités vis-à-vis des processus climatiques environnants. En effet, plusieurs projections ont montré que la zone de convergence intertropicale pourrait se déplacer vers le sud dans le futur (Rauscher et al., 2011;Hidalgo et al., 2013). Cette région délimite la convergence des alizées des hémisphères Nord et Sud, et provoque les fortes précipitations connues actuellement. Son déplacement vers le Sud pourrait donc entraîner des sécheresses accrues dans le Nord de l'Amérique Centrale au Guatemala, au Honduras (Figure 30), et dans la moitié Nord du Nicaragua, et des précipitations plus élevées dans le Sud au Panama, mais peu de changements entre les deux au Costa Rica ou dans la moitié Sud du Nicaragua (Hidalgo et al., 2016;Imbach et al., 2017).



**Figure 30.** Différence entre la pluviosité annuelle (mm) simulée durant la période 2029-2049 (moyenne de 7 modèles) et mesurée pendant la période historique 1979-1999. Gauche : RCP4.5, droite : RCP8.5. Les pays du Nord au Sud sont : Guatemala et Belize (Nord-Est), Honduras, El Salvador, Nicaragua, Costa Rica et Panama. Figure adaptée depuis Hidalgo et al. (2016).

Il est aussi important de noter que les simulations de changements climatiques dans notre travail n'appliquaient que des tendances moyennes à l'échelle du mois, mais ne modifiaient pas la variabilité à l'intérieur des mois ou des journées, ni n'ajoutaient d'effets extrêmes en plus de ceux présents dans les données mesurées (et éventuellement amplifiées via les tendances des GCM). Or, les changements climatiques risquent d'augmenter la probabilité d'évènements extrêmes tels que les pics de chaleurs ou le nombre de jours sans pluie (Barros et al., 2014). De plus, bien que les tendances simulées soient issues d'une moyenne de plusieurs

modèles choisis pour leur meilleure représentation des conditions actuelles grâce à l'intégration de facteurs importants tels que l'ENSO (Oscillations australes d'El Niño), les ensembles de prédictions des différents modèles contiennent eux-mêmes une certaine variabilité, sans même parler de l'effet que les conditions initiales peuvent avoir sur les prédictions de chacun (Hawkins et al., 2016).

Cependant, notre méthodologie a l'avantage de donner une information résumée, plus simple à appréhender et à utiliser par la suite dans les modèles de croissance de plantes, même si la prévision des impacts des changements climatiques doit par la suite être relativisée en rapport avec la variabilité des prédictions, et les incertitudes des modèles. Mais l'interprétation de nos résultats ne devrait se faire que dans le sens du "pire", car les impacts seront probablement plus négatifs que prévus, car comme le montrent Lewandowsky et al. (2014), une plus grande incertitude est associée à des dommages plus importants. Ils ajoutent aussi que l'incertitude doit appeler à une plus forte inquiétude (plutôt que plus faible), car celle-ci grandit plus vite vers les scénarios non désirés que vers les scénarios acceptables.

## 5.2. Méthode de simulation des plantations pérennes hétérogènes

### 5.2.1. Les processus environnementaux importants

Certains processus sont plus influencés que d'autres par la conjonction des effets des changements climatiques et de la gestion. Il est donc important que ces processus soient modélisés dans les PBM, mais aussi que leur représentation soit faite avec précision et justesse. Nous développons ici quelques-uns des processus qui nous apparaissent indispensables à bien modéliser, en détaillant les causes de leur choix, et en rappelant comment nous avons intégré leur effet dans notre méthodologie de modélisation.

#### *La lumière*

La lumière est la seule source d'énergie externe au système, et contrôle les bilans d'énergie, de carbone et d'eau des plantes et du sol. Les différentes gestions des arbres telles que l'élagage, l'éclaircie, la croissance libre ou l'émondage ont toutes un effet bien particulier sur l'interception de la lumière de l'écosystème. Par exemple l'éclaircie aura tendance à laisser de grandes trouées là où étaient positionnés les arbres coupés et donc à augmenter l'hétérogénéité spatiale de la distribution de la lumière au sous-étage, alors que l'émondage d'arbres plantés en plus grande densité au-dessus d'une culture va plutôt augmenter l'hétérogénéité de la lumière pendant une courte période suivant la période d'émondage. Aussi, les plantations agroforestières tendent à présenter des densités d'arbres d'ombrage relativement faibles à la plantation pour les gestions à croissance libre. Considérer l'interception lumineuse à l'échelle de la parcelle a tendance à sous-estimer la transmittance des arbres d'ombrage à cause de l'effet combiné d'une forte fraction de trous entre les couronnes et du regroupement des feuilles à l'intérieur des couronnes des arbres, qui laissent passer beaucoup plus de lumière qu'une canopée considérée homogène (Luedeling et al., 2016). De plus, la réponse de la photosynthèse à la lumière absorbée n'est pas linéaire car elle sature pour de fortes luminosités à cause de limitations biochimiques (*i.e.* vitesse de carboxylation de la Rubisco, voir modèle de Farquhar et al. (1980)

pour plus de détails). La non-linéarité de la réponse de la photosynthèse à la lumière implique que la photosynthèse à l'échelle de la parcelle ne pourra pas être retrouvée en simulant un arbre moyen, mais plutôt en moyennant toutes les photosynthèses des plantes de la plantation. Quantifier précisément la quantité de lumière absorbée par la culture est donc primordial pour modéliser l'effet de la gestion des arbres.

Dans notre étude, le modèle 3D MAESPA a été utilisé pour simuler l'interception de la lumière à l'échelle de chaque arbre, et même à l'échelle du voxel (partie homogène de la couronne). Le modèle a été validé précédemment dans une étude de Charbonnier et al. (2013) sur le système agroforestier d'Aquières, puis testé de nouveau dans le Chapitre 2 sur le système agroforestier d'Aquières et sur une plantation clonale d'Eucalyptus (le Maire et al., 2013), et enfin sur un essai agroforestier plus complexe, comportant de nombreuses conformations d'arbres d'ombrages, plantés seuls ou en mélange de deux espèces, avec une gestion en croissance libre ou émondée. MAESPA a donné des résultats satisfaisants (DIFN RMSE de 0.08, où DIFN est la fraction de diffus non-interceptée, un proxy de la canopy openness), et peu biaisés par l'effet d'ombrage. Dans un deuxième temps, la transmittance des arbres a été calculée en utilisant des coefficients d'extinction de la lumière directe et diffuse issus de métamodèles de MAESPA. L'utilisation de ces coefficients aux côtés d'un métamodèle de calcul de la LUE depuis MAESPA ont ainsi permis de prendre en compte indirectement l'effet de l'hétérogénéité spatiale du système agroforestier à l'échelle de la parcelle par notre modèle de croissance.

### *La température*

La température est le premier facteur impacté par les changements climatiques, et celui pour lequel l'incertitude est la plus faible, car les processus en jeu sont plus simples à appréhender que par exemple ceux impactant la pluviométrie ou les courants marins. Elle influe sur de nombreux processus, tels que la photosynthèse, la transpiration, la respiration, l'évaporation, ou encore sur les stades phénologiques de la plante dont le développement végétatif et la reproduction. A son tour, la température d'une plante dépend de son bilan d'énergie. Une plante peut absorber de l'énergie en absorbant de la lumière, ou plus rarement par des flux négatifs d'énergie sensible en équilibrant sa température avec celle de l'atmosphère si cette dernière est plus chaude, comme la nuit par exemple. Elle pourra ensuite perdre de l'énergie par deux moyens : l'énergie latente qui est caractérisée par la transpiration et l'évaporation de l'eau de pluie à sa surface ; et par un échange positif d'énergie sensible, en équilibrant sa température avec celle de l'atmosphère si cette dernière est plus froide. Chacun de ces flux est lui-même influencé par d'autres facteurs. Par exemple, la transpiration va dépendre de l'état hydrique de la plante, mais aussi de la conductance entre les stomates et l'air à la surface des feuilles. Il existe donc dans la zone proche de la feuille un volume d'air dans lequel la feuille a une forte influence par sa transpiration et sa température, que l'on appelle aussi couche limite. Sa taille peut être réduite par le vent, qui va donc faciliter les flux d'énergie latente et sensible entre la plante et l'atmosphère. Pour résumer, si la plante absorbe plus d'énergie qu'elle n'en dissipe, alors sa température intrinsèque augmentera,



et vice et versa. Donc, la température d'une plante dépend de la lumière qu'elle absorbe, de sa transpiration, de la température de l'air à sa proximité, et du vent.

Les changements climatiques vont augmenter la température de l'air dans la couche basse de l'atmosphère par effet de serre, et donc augmenter la demande évaporative. Si la plante n'est pas limitée en eau, sa transpiration va donc augmenter, mais si elle est en stress hydrique et qu'elle ferme ses stomates, sa température de canopée va alors augmenter. La gestion, et notamment l'agroforesterie pourra abaisser les extrêmes de températures (chaud le jour, froid la nuit) en diminuant la demande évaporative et en réduisant l'énergie disponible pour les plantes cultivées en sous-étage. En revanche, l'agroforesterie va aussi abaisser la vitesse du vent, ce qui va diminuer la conductance, et donc diminuer les échanges d'énergie entre la canopée et l'atmosphère.

La température de canopée des plantations a été calculée en utilisant une version modifiée de MAESPA, comme décrit dans le Chapitre 2. En effet, cette version a été adaptée en ajoutant une étape de plus dans le calcul de la température de canopée. Cette étape passe par un calcul de la température de l'air à l'intérieur de la canopée, qui peut être très différent de celui des couches basses de l'atmosphère au-dessus de l'écosystème, spécialement lors de vents faibles, ou lorsque la canopée est dense. Le calcul de l'extinction du vent a aussi été revu pour intégrer un profil de vent modulé par la présence du sous-étage, pour mieux représenter l'effet de chaque strate sur le vent. MAESPA a ensuite été comparé pour ses simulations de température de canopée avec des mesures faites sur différentes gestions de l'ombrage. Similairement à l'interception de la lumière, la température de canopée a ensuite été intégrée au modèle dynamique de culture au travers de métamodèles issus de MAESPA pour bénéficier d'un calcul prenant en compte l'hétérogénéité spatiale des parcelles, tout en donnant un résultat à l'échelle de la parcelle.

#### *Le déficit de pression de vapeur, et la transpiration*

Le déficit de pression de vapeur (VPD) est calculé à partir de la différence entre l'humidité de l'air et la pression de vapeur saturante de l'eau. Le VPD est impacté positivement par l'augmentation de la température de l'air. En effet, plus l'air est chaud, plus celui-ci peut contenir d'eau avant saturation. Ce facteur environnemental est un proxy de la demande évaporative de l'air, et impacte directement la transpiration. En effet, plus le VPD est haut, plus la plante aura tendance à transpirer. Lorsque le VPD est trop grand, celui-ci peut faire chuter (négativement) dangereusement le potentiel foliaire à cause d'une trop grande demande évaporative comparé à la conductivité hydraulique de la plante et au potentiel hydrique du sol, ce qui peut entraîner des cavitations. Certaines plantes ferment donc leurs stomates pour éviter ces effets, et maintenir un potentiel foliaire adéquat. Au contraire, un VPD trop faible peut limiter la possibilité de la plante à transpirer, et peut avoir des conséquences sur sa température, et peut aussi favoriser le dépôt d'eau à la surface des feuilles, ce qui va augmenter la probabilité de développer des maladies (Huber and Gillespie, 1992). Il est probable que le VPD soit positivement impacté par les changements climatiques à cause de l'augmentation de la température de l'air. Toutefois, la gestion des arbres peut aussi modifier le VPD à l'intérieur de la canopée.

Par exemple, les AFS auront tendance à diminuer le VPD en diminuant la température, et en augmentant l'humidité de l'air.

Bien modéliser la demande évaporative va donc de pair avec la modélisation de la température. C'est pourquoi MAESPA a aussi été modifié pour calculer la pression de vapeur à l'intérieur de la canopée (Chapitre 2). Ce calcul a été inclus dans le modèle dynamique de culture via l'utilisation de métamodèles pour simuler directement la transpiration.

### *Le vent*

Le vent favorise les flux entre la plante ou le sol et l'atmosphère via son impact sur la conductance des couches limites au niveau de la feuille, du sol ou de la canopée. Il va donc avoir un effet fort sur la transpiration, ainsi que sur la température des plantes. Des vents excessifs peuvent aussi endommager les plantations. L'effet des changements climatiques sur les vents est très incertain (Solomon et al., 2007), mais la gestion peut diminuer leur force (Luedeling et al., 2016) ainsi que les impacts des tempêtes (Blennow et al., 2010; Lin, 2011).

Dans MAESPA, le vent est une variable de forçage, mais sa vitesse a été modifiée à l'intérieur de la canopée en utilisant un modèle de profil de vent calibré sur des données mesurées. Le modèle dynamique de culture ne différencie pas de vitesse de vent différente entre les couches simulées. Cependant, les variables influencées par le vent comme la transpiration, la photosynthèse ou les flux sensibles sont toutes issues de métamodèles de MAESPA, qui prennent eux-mêmes en compte les effets de la structure des plantations.

### *La concentration en CO<sub>2</sub> atmosphérique*

La concentration en CO<sub>2</sub> atmosphérique peut avoir un fort impact sur la photosynthèse des plantes. Dans le cas d'une plante non limitée par un autre facteur, augmenter la concentration en CO<sub>2</sub> atmosphérique augmentera l'assimilation de CO<sub>2</sub>. Un effet indirect de cette augmentation est que la plante perdra moins d'eau pour obtenir une même assimilation de carbone, elle augmentera donc son efficacité d'utilisation de l'eau, ce qui peut diminuer l'impact des sécheresses (Hatfield et al., 2011). Le CO<sub>2</sub> peut donc compenser l'effet négatif de l'augmentation de la température et du VPD sous changement climatique. Dans MAESPA le modèle de photosynthèse foliaire utilisé (Farquhar et al., 1980) permet de simuler l'effet positif du CO<sub>2</sub> sur la photosynthèse. Dans le modèle dynamique de culture, l'effet du CO<sub>2</sub> est inclus dans le métamodèle de MAESPA pour le calcul de l'efficacité d'utilisation de la lumière.

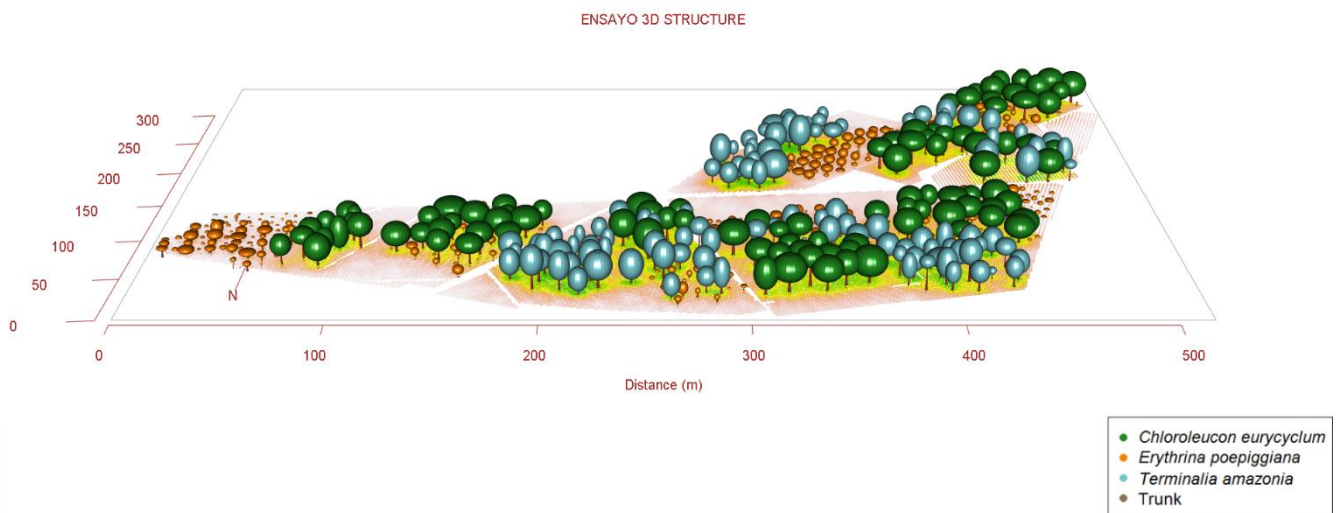
### **5.2.2. L'échelle de travail**

Les effets d'échelles sont importants à prendre en compte dans la modélisation des plantations pérennes qui présentent des structures complexes, car certains processus ne sont pas linéaires. On peut voir par exemple dans la Figure 31 que la lumière diffuse qui arrive jusqu'à la couche de caféier est extrêmement variable d'une plante à l'autre. En effet, certains individus ne sont jamais sous ombrage, d'autres le sont toute la journée, et d'autres encore le sont plus ou moins de façon épisodique. De plus, l'ombrage est en fait issu du rayonnement

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incident, qui est une variable continue, et qui dépend non seulement de la lumière directe, mais aussi de la lumière diffuse, qui peut être particulièrement importante pour des régions où il y a souvent une forte couverture nuageuse.

Par conséquent, connaître l'interception de la lumière par les arbres d'ombrages à l'échelle de la parcelle requiert de calculer la somme des interceptions de chaque individu. Ceci est d'autant plus vrai que l'hétérogénéité de la parcelle augmente, comme dans les AFS ayant des densités d'arbres d'ombrage faibles tels qu'à Aquiares (Charbonnier et al., 2013). De plus, de nombreux processus dépendent ensuite du rayonnement incident (global ou PAR), comme nous l'avons décrit plus haut (paragraphe 5.2.1).



**Figure 31. Représentation tridimensionnelle de l'essai agroforestier du CATIE au Costa Rica. La fraction de diffus interceptée par la canopée des arbres d'ombrages est projetée à hauteurs de la couche des caféiers (2m du sol), et son intensité est dénotée par la couleur des points : vert pour une forte interception, rouge pour une interception faible, blanc pour aucune interception.**

Cependant, prendre en compte des processus fins peut demander l'utilisation de modèles complexes, qui ne sont parfois pas adaptés à l'échelle de calcul désirée : temps de calcul, complexité de leur paramétrage, difficulté du couplage, etc... Ainsi, nous avons proposé une méthode de couplage de modèles utilisant des métamodèles dans le Chapitre 3 et le Chapitre 4. Cette méthode, qui a été simplifiée par rapport à ce qui peut exister dans la littérature (Christina et al., 2016; Faivre et al., 2013; Villa-Vialaneix et al., 2012) nous a permis de prendre en compte les effets d'échelles fines (individu) dans un modèle à plus grande échelle (parcelle), tout en gardant un taux d'erreur acceptable ( $R^2$  systématiquement supérieurs à 0.85 sauf pour une variable).

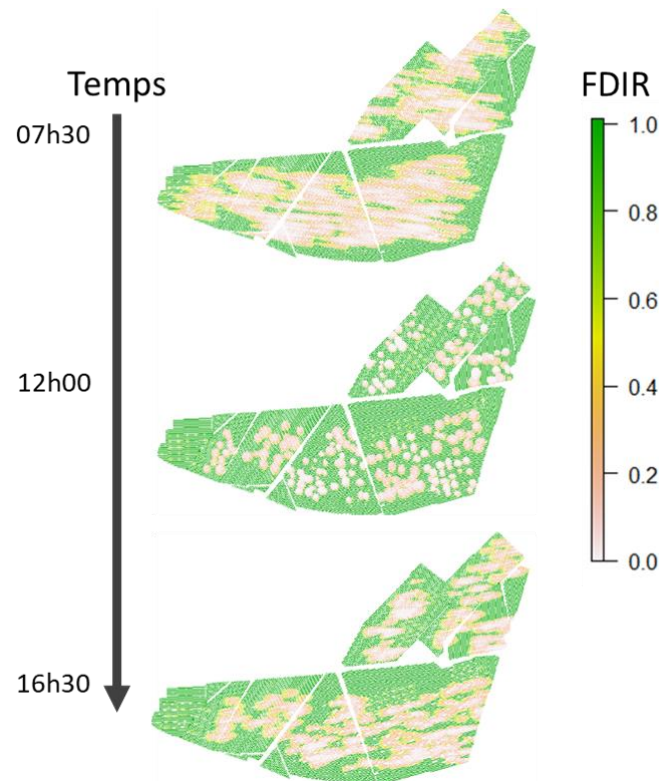
### 5.2.3. Les modèles

Comme décrit dans le paragraphe 1.3 de ce manuscrit, il existe de nombreux types de modèles simulant les plantations pérennes. Mais pour prendre en compte tous les effets de toutes les gestions possibles (éclaircie, dépressage, élagage, agroforesterie...), un modèle idéal intégrerait les processus à toutes les échelles spatiales, depuis la plante jusqu'au paysage. Ce modèle idéal devrait aussi être rapide d'exécution pour pouvoir simuler

plusieurs rotations entières de la culture à l'échelle de la parcelle, de la région, voire du globe pour permettre de simuler l'effet des changements climatiques sur la plantation.

Cependant, nous insistons ici sur le fait que, si certains modèles prennent en compte les différents processus importants que nous avons cité (voir Porté and Bartelink (2002), Fontes et al. (2010) ou plus récemment Pretzsch et al. (2015) pour une revue des modèles), aucun n'a la capacité de calculer à la fois les effets de toutes les gestions possibles, et les effets des changements climatiques aux échelles spatiales et temporelles auxquelles ils agissent. Nous adhérons ainsi aux conclusions présentées par Pretzsch et al. (2015), qui exposent le fait que de nombreux modèles sont présentés comme ayant la possibilité de prendre en compte les effets de gestion tels que le mélange d'espèces, mais qu'ils contiennent en réalité trop souvent des modules simplifiés qui ne représentent pas de façon réaliste les processus qui influent réellement le système. Ils ajoutent aussi qu'il est important de considérer que le fait qu'un modèle prédit la croissance avec précision ne signifie pas qu'il le fait pour les bonnes raisons physiologiques, car beaucoup de modèles sont en fait ajustés empiriquement (*i.e.* tuned) jusqu'à obtenir de bonnes prédictions, ce qui les rends non génériques. Or les changements climatiques et les changements de gestion risquent d'influencer non-linéairement les processus d'eau, d'énergie et de carbone, qui ne seront alors plus bien représentés par le modèle car il ne décrit pas complètement le système. Ce constat est probablement issu du fait qu'il existe toujours un compromis entre la rapidité d'exécution et la finesse des processus.

Par exemple, parmi les dizaines de modèles potentiels qui auraient pu être utilisés dans cette thèse, le modèle BALANCE (Grote and Pretzsch, 2002) est probablement celui qui se rapprochait le plus de nos objectifs. Celui-ci prend en compte les effets critiques décrits précédemment, et a déjà été testé avec succès sur des mélanges d'espèces (Rötzer et al., 2010). Cependant, même s'il décrit la parcelle à l'échelle de l'arbre, il ne prend pas en compte les effets intra-journaliers de la distribution de lumière, qui peuvent être relativement forts dans des systèmes de grande complexité structurelle comme les AFS (Charbonnier et al., 2013) comme on peut le voir dans la Figure 32.



**Figure 32.** Projection 2D (vue par le haut) d'une simulation de la fraction de lumière (PAR) directe transmise à hauteur de caféier (2 m), en fonction de l'heure de la journée dans l'essai agroforestier du CATIE au Costa Rica, pour une journée ensoleillée. Le modèle utilisé est MAESPA. La projection de l'ombre de la canopée des arbres d'ombrage change avec la position du soleil. Certains caféiers ne sont jamais impactés par l'ombrage dans les parcelles plein soleil, d'autres le sont toute la journée sous les arbres, et d'autres enfin ne le sont que le matin ou que l'après-midi.

La méthode de modélisation que nous avons utilisée consiste à utiliser deux modèles à échelles de travail différente, et à les coupler. Un premier modèle basé sur des processus à l'échelle de la plante et décrivant la structure de la canopée en 3D (MAESPA), et un deuxième modèle basé sur des processus à l'échelle de la parcelle pour calculer les stades de développement de la plantation. Les deux modèles sont ensuite couplés grâce à l'utilisation de métamodèles qui résument les calculs du premier en un jeu simple d'équations, et qui sont ensuite intégrés dans le deuxième modèle.

Ainsi, nous avons d'abord modifié MAESPA pour lui permettre de mieux prendre en compte les effets de température et de pression de vapeur à l'intérieur de la canopée pour mieux simuler les températures de canopée, et donc par la suite les bilans d'énergie, d'eau et de carbone (Chapitre 2). Nous avons ensuite développé un modèle dynamique de culture basé sur plusieurs autres modèles. Les différentes phases de développement sont dérivées des modèles de Rodríguez et al. (2011) ainsi que de Van Oijen et al. (2010b), et les calculs du sol proviennent du modèle BILJOU (Granier et al., 2012). Notre méthodologie de simulation nous a ainsi permis de développer et d'utiliser rapidement un modèle capable de simuler à la fois les effets de la gestion et les effets des changements climatiques sur les plantations pérennes étudiées.

## 5.3. Effet de l'ombrage sur les plantations de café

### 5.3.1. Lumière et température

Bien simuler la lumière dans un système à structure complexe est primordial (Charbonnier et al., 2013). D'une part, elle est le seul composant extérieur qui apporte de l'énergie au système, et d'autre part, les processus d'interception, de réflexion et de transmittance peuvent engendrer de grandes disparités dans un système (Figure 31 et Figure 32). En effet, dans notre étude sur l'essai agroforestier du CATIE, la fraction de lumière diffuse mesurée en moyenne par traitement s'étendait du simple au double, de 42% à 87%, montrant une grande hétérogénéité entre gestions. De plus, la variance de la transmittance à l'intérieur des traitements est fortement liée à l'hétérogénéité induite par la gestion, avec des valeurs très faibles en plein soleil (variance= 0.051%, écart-type= 2%), et très fortes sous systèmes complexes comme les mélanges d'espèces (écart-type= 26%). Utiliser un modèle à l'échelle parcelle demanderait donc au moins un paramétrage de chaque gestion différente pour prendre en compte les variations entre gestions, et ne pourrait pas rendre compte de la forte variabilité spatiale à l'intérieur même de chaque parcelle. De plus, la lumière directe transmise à chaque caféier par la canopée d'arbres d'ombrage peut beaucoup varier dans la journée, augmentant ainsi la variabilité de la lumière totale reçue par chaque plante. Nous avons relevé des écart-types à l'intérieur de la journée allant jusqu'à 26% de la lumière transmise au-dessus d'un seul caféier entre différentes heures. Un modèle fonctionnant à l'échelle de la journée ne pourrait donc pas prendre en compte la forte hétérogénéité temporelle induite par la gestion.

La température des feuilles est elle aussi calculée pour chaque individu via son bilan d'énergie qui dépend lui-même de la lumière absorbée par la plante (et de sa température aussi). Ces calculs suivent donc le même schéma que la lumière, c'est-à-dire que l'hétérogénéité spatiale et temporelle de la température est bien prise en compte. Ce processus est important car la température contrôle à son tour de nombreux facteurs physiologiques comme la photosynthèse, la transpiration, la respiration de maintenance ou encore la phénologie.

Toutefois, certaines améliorations pourraient être apportées quant au paramétrage de nos systèmes d'études pour la simulation des températures de canopée, notamment en intégrant les compartiments ligneux qui étaient jusqu'alors absents (sauf les troncs des arbres d'ombrage), et qui pourraient avoir un effet substantiel au travers de l'accumulation de rosée notamment. Cependant, la nouvelle version de MAESPA simule relativement bien la température de canopée en comparaison avec les modèles existants tels que celui de Bailey et al. (2016) ou le modèle SHAW (Flerchinger et al., 2015).

L'utilisation du modèle 3D MAESPA permet donc d'étudier l'effet de la variabilité intra-parcellaire de lumière et de température, ce qui autorise une prise en compte des réponses non-linéaires d'autres variables dont la photosynthèse. Cette méthode permet de mieux représenter les effets de la gestion et des changements climatiques à fine échelle, là où ils auront probablement le plus d'importance.

### 5.3.2. Evapotranspiration

Les systèmes agroforestiers ont tendance à réduire l'évaporation de l'eau du sol (Holwerda et al., 2013; Wallace et al., 1999), et à réduire la transpiration des caféiers (Lin, 2010).

Nos simulations de l'évapotranspiration des caféiers ont montré qu'aucun système n'était limité par la disponibilité en eau sur nos sites, mais que la gestion et le climat ont un fort impact sur le bilan hydrique. En effet, les caféiers en plein soleil sous climats chauds transpirent en moyenne deux fois plus que ceux sous ombrage élevé. Cet effet montre que les caféiers ont une plasticité relativement grande quant aux conditions microclimatiques et de lumière auxquels ils sont sujets, du moins tant que la disponibilité en eau n'est pas limitante. Cependant, la transpiration des arbres d'ombrage de la plantation AFS du CATIE est tellement élevée que l'évapotranspiration de cette parcelle est deux fois supérieure à celle de la culture en plein soleil. Toutefois, AQUIARES et CATIE sont deux sites ayant des pluviométries élevées (2816 mm au CATIE, 3144 à AQUIARES) qui dépassent toujours deux fois les valeurs d'évapotranspirations des AFS. Le site de TARRAZU présente quant à lui un climat plus sec, mais aussi des températures plus faibles, ce qui permet aux plantations de conserver une évapotranspiration toujours largement inférieure aux précipitations, qu'elles soient en plein soleil ou en AFS. Il est donc important de souligner que les bilans hydriques sont très variables entre plantations, et que la gestion et le climat sont deux facteurs à forte influence. En somme, il faut garder à l'esprit que nos prédictions ne peuvent pas être généralisées comme telles à d'autres régions de cultures du café qui pourraient avoir un climat plus sec et plus chaud, car nos simulations n'ont pas été effectuées sur des sites ayant les deux à la fois. Il serait intéressant toutefois d'appliquer notre modèle à de telles conditions pour étudier l'effet de la gestion sur l'évapotranspiration en conditions de stress hydrique.

### 5.3.3. Flux de chaleurs sensibles et latents

Les simulations ont montré que le partitionnement de l'énergie sensible et latente est fortement impacté par le taux d'ombrage. En effet, les parcelles cultivées en plein soleil présentent un partitionnement de l'énergie totale annuelle à peu près équivalent entre flux de chaleur sensible et latent, voire plus élevé pour les flux sensibles, alors que les parcelles AFS présentent une distribution de l'énergie beaucoup plus forte en faveur du flux de chaleur latent. Les AFS modifient ainsi le microclimat de la plantation vers des températures de canopée des plantes de sous-étages et du sol plus fraîches, un air plus humide et une radiation moins intense. Ces conditions peuvent bénéficier à la culture de caféier pour des conditions suboptimales comme au CATIE qui présente une température annuelle moyenne élevée pour la culture du café arabica, et pour diminuer la variabilité de la production de café (Lin, 2007). Cet effet de partitionnement est principalement dû à une plus forte évapotranspiration dans les parcelles AFS qu'en plein soleil grâce à une meilleure régulation stomatique et d'un LAI total plus élevé. Des résultats similaires de partitionnement de l'énergie ont aussi été mesurés sur un AFS de café au Mexique (Holwerda et al., 2013), avec un ratio de Bowen à environ 0.5, soit des valeurs deux fois supérieures de flux latents que de flux sensibles.

### 5.3.4. La production de café

Il est souvent avancé que le rendement des cultures de café peut être négativement impacté par l'augmentation de l'ombrage, notamment à cause de : (1) une réduction de la photosynthèse à cause de la réduction de lumière transmise, même si l'efficacité de l'utilisation de la lumière peut compenser la perte de lumière dans les plantations à faible densité d'arbres d'ombrage (Charbonnier et al., 2017) ; (2) une réduction du nombre de nœuds porteurs de fleurs (DaMatta et al., 2007) à cause de la réduction de la température, et donc de la croissance végétative. Cependant, l'ombrage réduit aussi la radiation, ce qui impacte positivement l'apparition de bourgeons floraux (Rodríguez et al., 2011), et améliore les qualités gustatives du café grâce à une période de maturation plus longue et plus synchronisée (Muschler, 2001; Vaast et al., 2006). La période de maturation plus longue permet au fruit d'accumuler plus de sucres dans la graine (Pezzopane et al., 2012), et une maturation synchronisée permet de diminuer le nombre de fruits immatures à la récolte qui produisent des cafés plus amer, astringent et de qualité inférieure (Vaast et al., 2006; Farah et al., 2006).

Sous conditions climatiques actuelles, et sur les sites d'Aquiaries et de Tarrazu, notre modèle ne montre pas d'effet de l'ombrage sur la production, sauf pour la gestion AFS sous *Cordia alliodora* en gestion de référence (*i.e.* éclaircie dès que les arbres interceptent plus de 30% de la lumière), qui montre une augmentation légère de la moyenne de production (*c.a.* 2%). Toutefois, plus de sites et de gestions doivent être testés, car ces deux sites présentent des climats bien particuliers, où les caféiers sont dans des conditions climatiques actuelles encore adaptées pour la production de café malgré leur basse altitude. De plus, notre modèle doit encore être validé plus précisément pour chaque processus pris en compte, et notamment pour le développement reproductif pour lequel nous manquons de données, et qui pourtant est probablement le plus difficile à modéliser en utilisant des équations mécanistes car il dépend de nombreux processus, et s'étend sur deux ans (Camargo and Camargo, 2001). Néanmoins, les valeurs globales de productions simulées par le modèle sont tout de même dans la gamme des productions relevées sur le site d'Aquiaries (Charbonnier et al., 2017) et de Tarrazu (Meylan, 2012). De plus, le modèle prédit des variations interannuelles de production plus fortes à Tarrazu comparé à Aquiaries, et la gamme de variation simulée est en accord avec ce qui a pu être mesuré par Meylan (2012).

## 5.4. Effets des changements climatiques sur la production de café

### 5.4.1. Effets des changements climatiques

Les effets des changements climatiques sur la culture du caféier vont avant tout dépendre du climat actuel de chaque localité. En effet, une culture de caféier plantée aujourd'hui en haute altitude va probablement avoir une plus grande production sous températures plus élevées si les caféiers étaient en conditions suboptimales. Au contraire, une culture plantée en basse altitude, déjà à la limite des climats tolérés par la plante, aura probablement des productions encore plus faibles. Cependant, l'augmentation de la température de l'air va aussi s'accompagner d'une augmentation de la concentration en CO<sub>2</sub> atmosphérique, dont l'effet est positif sur la photosynthèse, ou au moins neutre (Ellsworth et al., 2017). L'interactions de la température et du CO<sub>2</sub> peut



donc être complexe, car leurs effets peuvent être antagonistes parfois (*e.g.* basse altitude), comme tout deux positifs (*e.g.* haute altitude). Ce fut en effet le cas dans les résultats de nos simulations sur Aquiares et Tarrazu, deux sites aux altitudes et aux climats différents.

Les conditions climatiques optimales pour le développement du café se situent entre 18°C et 21°C pour la température annuelle moyenne, et 1200 à 1800 mm pour les précipitations (DaMatta and Ramalho, 2006). Les deux sites observés sont dans la fourchette haute de la gamme de température, avec 19.4°C à Aquiares, et 18.0°C à Tarrazu. En conséquence, notre modèle prédit qu'une augmentation de la température seule aurait un effet négatif sur la NPP dans les deux sites (-11.2%). Cependant, l'augmentation de la concentration de CO<sub>2</sub> atmosphérique compense, et même dépasse largement l'effet négatif de l'augmentation de température dans les simulations, pour donner finalement une NPP plus élevée sous les conditions climatiques futures prédites dans ces deux sites (*c.a.* +26% à l'horizon 2100). Néanmoins, l'augmentation de la NPP n'est pas suivie par une augmentation de la production de grains de café. Le modèle montre que l'offre en carbohydrates est déjà suffisante dans le modèle en climat actuel, et donc que son augmentation n'est pas corrélée avec une augmentation de la production de fruits. Au contraire même, l'augmentation de température diminue progressivement la production de fruits entre 1979 et 2100 à Aquiares (-40%) malgré l'augmentation de la NPP. Cet effet d'indépendance apparente entre NPP et production de fruits provient entre autres, dans le modèle, de la distribution temporelle de la demande en carbone des fruits qui est étalée dans le temps, ce qui permet au caféier de conserver des réserves de carbohydrates relativement élevées même en période de remplissage des grains.

Les précipitations annuelles à Tarrazu (1662 mm) semblent être dans la gamme optimale (1200 à 1800 mm), alors que celles d'Aquiares sont plus élevées, avec 2767 mm par an répartis uniformément le long de l'année (seulement un mois de relative sécheresse en avril, alors que Tarrazu à une saison sèche plus marquée). Or, les caféiers ont besoin d'une période sèche d'une durée de 2 à 4 mois pour optimiser et regrouper la levée de dormance des bourgeons (Haarer, 1956). Donc moins le caféier est sujet à des stress hydriques pendant la dormance, moins les levées de dormances seront regroupées, et plus la demande en carbone liée à la croissance des fruits sera étalée dans le temps. Une demande en carbone étalée dans le temps permet aussi une utilisation plus partagée des réserves pour la croissance des fruits ou pour l'appareil végétatif. Il a été montré que les ressources disponibles pour les organes végétatifs du caféier tels que les feuilles, les racines et les branches peuvent être fortement impactées par la croissance des fruits qui est prioritaire, ce qui peut ensuite affecter leur production et leur santé (DaMatta et al., 2007). Ce phénomène est bien représenté par le modèle, mais il est peut-être sous-estimé car les réserves du caféier sont certes fortement impactées par le développement reproductif, mais retombent rarement à zéro dans nos simulations, même à Tarrazu qui a pourtant des réserves plus faibles. Le phénomène d'étalement dans le temps de la production des fruits explique la relative constance de production simulée et observée à Aquiares comparativement à Tarrazu. Cependant la production en est légèrement impactée car moins de bourgeons éclosent au total, ce qui est aussi noté par DaMatta and Ramalho (2006).

Nous pourrions alors simplement conclure que les changements climatiques auront un effet négatif sur la production de café, car seul l'effet négatif de l'augmentation de la température influence la production à Aquiares. Néanmoins, ce n'est pas le cas à Tarrazu, où le modèle prédit d'abord une augmentation de la production de café entre 2020 et 2050, même si la variabilité interannuelle de production augmente fortement. Là aussi, cet effet d'augmentation semble indépendant de la NPP comme à Aquiares, et seulement lié à l'augmentation de température, qui était suboptimale pour le développement reproductif jusqu'alors. Ensuite, le modèle prédit que l'augmentation de température réduit sérieusement la production (-50%) sur la période 2060-2100 comparativement à la période 1979-2020.

Une validation sur un jeu de données plus explicite sur les phases de développement phénologique est donc indispensable pour savoir si ces effets sont bien représentés par le modèle, ou si les conditions climatiques des deux sites permettent réellement de limiter l'épuisement des réserves. C'est d'ailleurs particulièrement le cas à Aquiares où l'apparition des fruits est très progressive, ce qui permet une meilleure répartition de la demande en carbone sur le temps et évite donc une trop forte compétition pour le carbone entre les différents organes.

De plus, il est important de souligner que le modèle n'intègre aucun effet d'acclimatation à l'environnement telle que la régulation de l'effet d'augmentation du CO<sub>2</sub> sur la photosynthèse, et ne prends pas en compte l'effet de l'ozone ou des nutriments, qui peuvent avoir un effet substantiel sur la production (Constable and Friend, 2000; Hatfield et al., 2011). Cependant, les simulations sur l'effet du CO<sub>2</sub> et de la température sont en accord avec les observations faites par Rodrigues et al. (2016), qui montrent que l'effet CO<sub>2</sub> compense et dépasse l'effet de la température sur la photosynthèse. De plus, il semblerait que *C. arabica* ne présente pas d'effet de régulation de l'effet du CO<sub>2</sub> dans la nature (DaMatta et al., 2016), donc son absence dans le modèle n'est pas un problème. Enfin, les caféiers sont souvent fortement amendés, avec par exemple plus de 200 kg N ha<sup>-1</sup> Y<sup>-1</sup> à Aquiares (Charbonnier et al., 2017), et continueront probablement à l'être dans le futur, ce qui réduit l'erreur de la disponibilité en nutriment par la plante sur nos simulations.

Jusqu'à aujourd'hui, de nombreuses études ayant pour objectif de prévoir les effets des changements climatiques sur la production de café sont basés sur des modèles empiriques, incluant ou non explicitement les effets de la température et du CO<sub>2</sub>. Un premier exemple se trouve dans le travail de Verhage et al. (2017), qui utilisent une adaptation du modèle de Camargo et al. (2005) en y incluant un effet empirique du CO<sub>2</sub> comme un facteur d'augmentation de la production, et un effet de l'irrigation sur la température de canopée dérivé de données moyennes de productions de communes irriguées ou non. Un autre exemple est l'utilisation de modèles de distribution d'espèces tels que MaxEnt, qui calculent l'enveloppe environnementale de l'espèce (suitability) sur la base des localités où elle est présente, et appliquent cette enveloppe pour prédire la distribution de l'espèce sur des points inconnus, ou des climats futurs (Merow and Silander, 2014; Phillips et al., 2006). Ces modèles sont à la base utilisés pour calculer l'aire de répartition des espèces à l'état naturel, en partant du principe que leur distribution mesurée est résolue, c'est-à-dire qu'elle est représentative de l'ensemble des conditions possibles pour l'espèce. Utiliser ces modèles pour les cultures peut s'avérer délicat car la distribution d'une espèce cultivée peut dépendre d'autres facteurs comme de la gestion (agroforesterie,

irrigation etc...), qui ne sont pas forcément applicables dans toutes les zones de distribution. De plus, leur application à des conditions nouvelles est aussi très délicat car le modèle ne représente pas les processus, donc ne prend pas en compte leurs différentes interactions possibles en dehors de la gamme d'entraînement du modèle. Ils ne peuvent donc ni représenter l'effet des températures plus élevées sur un même emplacement, ni l'effet de fertilisation du CO<sub>2</sub>, mais ils ont pourtant été largement utilisés récemment par la communauté de modélisateur du café (Ovalle-Rivera et al., 2015; Bunn et al., 2015; Schroth et al., 2009; Baca et al., 2014; Läderach et al., 2017; Magrach and Ghazoul, 2015). Par conséquent, nous insistons sur le fait qu'il est fortement déconseillé de faire des prévisions de productions futures de café basées sur des modèles totalement empiriques, car d'une part les conditions climatiques futures sont absentes des conditions actuelles, c'est-à-dire qu'un modèle statistique ne peut pas être correctement entraîné sur les données actuelles ; et d'autre part car la production de café peut être indépendante de la production végétative sous certaines conditions, comme notre modèle le montre. Aussi, tout modèle est constitué d'équations empiriques à un certain point, donc la solution qui comporte le moins d'erreur est toujours l'expérimentation.

En somme, l'utilisation de modèles basés sur les processus apparaît donc indispensable pour prédire les impacts sur les différents facteurs en jeu (Constable and Friend, 2000; Pretzsch et al., 2015), car l'évolution future de la production de café dépendra principalement du climat actuel de la plantation et des interactions entre l'augmentation de CO<sub>2</sub>, de la température et des précipitations qui sont tous trois liés au rythme des changements climatiques (RCP4.5, 8.5...) pour un site donné.

#### 5.4.2. Adaptation par la gestion

Les avantages de l'ombrage sur les cultures de cafés sont très nombreux (paragraphe 5.3), et tout particulièrement sous conditions suboptimales (DaMatta et al., 2007). Ces avantages sont vrais tant que la gestion 1) optimise les effets positifs la réduction des températures extrêmes (Lin, 2007) ou la réduction de la radiation lors de l'initialisation des bourgeons, et 2) diminue les effets négatifs comme la perte de lumière qui est importante pour la photosynthèse (DaMatta et al., 2007). Les simulations du modèle de dynamique de culture montrent que l'ajout d'arbres d'ombrage *C. alliodora* en gestion de référence, c'est-à-dire avec des éclaircies dès que la transmittance est inférieure à 70%, peut être bénéfique sur les deux sites étudiés, avec une augmentation de 2% de la production, sans même compter les produits apportés par les arbres eux-mêmes (e.g. bois).

Ensuite, la gestion de l'ombrage a un effet de plus en plus bénéfique sur la production avec l'apparition du stress lié à l'augmentation de la température. En effet, non seulement la production est plus élevée dans les systèmes agroforestiers qu'en plein soleil, mais l'écart entre les deux augmente avec l'augmentation des températures. Pour optimiser les effets de l'ombrage pour les conditions futures, il est nécessaire d'augmenter l'ombrage, avec moins d'éclaircies pour les gestions en croissance libre de *C. alliodora*, ou moins de taille pour les gestions avec émondage comme *E. poeppigiana*. Il est intéressant de noter aussi que l'influence de chaque gestion sur la production diffère selon le climat : la gestion "Cordia adaptée" est toujours la meilleure

sauf à Tarrazu sous RCP4.5, "Erythrina adaptée" est la seconde meilleure sous trois scénarios, mais est la troisième à Aquiares sous RCP4.5, etc...

La gestion a le potentiel de compenser une partie des effets négatifs des changements climatiques à Aquiares et Tarrazu, mais elle doit être implémentée avec attention, car une mauvaise gestion peut aussi entraîner de grosses pertes de production à cause de la réduction de lumière transmise aux caféiers. Etant donné que la gestion et le CO<sub>2</sub> ne permettent pas une compensation totale de la perte de production de café due à l'augmentation des températures, d'autres outils d'adaptations devront donc être ajoutés, comme par exemple la sélection de cultivars plus résistants de hautes températures, comme celles utilisées au Brésil par exemple (DaMatta et al., 2007; DaMatta and Ramalho, 2006).

Enfin, il est à noter que les effets de l'ombrage pourraient être encore plus prononcés lors des changements climatiques. En effet, les projections climatiques utilisées n'ajoutent pas d'évènements extrêmes à l'échelle de la journée (minimum et maximum de température) ou de la saison (vagues de chaleurs), pourtant décrites comme très probables par le 5<sup>e</sup> rapport d'évaluation du GIEC (Barros et al., 2014). Or, les AFS sont particulièrement efficaces pour tamponner les extrêmes climatiques, comme les pics de chaleurs (Lin, 2007), ce qui pourrait donc encore ajouter de l'intérêt aux AFS par rapport aux cultures ouvertes.

## 5.5. Conclusion et Perspectives

Cette thèse aura permis de développer et de tester un modèle dynamique de culture du caféier qui prend en compte les effets liés à l'hétérogénéité spatiale des parcelles AFS grâce au couplage d'un modèle 3D basé sur les processus avec un nouveau modèle dynamique de culture à l'échelle de la parcelle par l'utilisation de métamodèles. Les originalités de ce travail sont multiples. En effet, notre modèle dynamique de culture est le premier modèle appliqué sur café qui prend en compte de nombreux effets liés à l'hétérogénéité spatiale. Les résultats des prévisions des effets des changements climatiques couplés aux effets de la gestion de l'ombrage sur les plantations de caféier sont donc pour l'instant unique.

Ce travail souligne le besoin crucial de données expérimentales sur les cultures pour paramétrer et valider les modèles, et en particulier pour le café dont le cycle reproductif est particulièrement complexe. Enfin, nous avons montré l'importance et l'urgence du développement de modèles basés sur les processus capables de les représenter à l'échelle où ils seront impactés par les changements climatiques, mais aussi par les différentes solutions d'adaptation pour qu'elles puissent être testées et donc implémentées plus tôt.

Le modèle 3D MAESPA a été modifié pour mieux représenter les effets du microclimat à l'intérieur de la canopée. Il a été paramétré et testé sur deux plantations agroforestières de café au Costa Rica ainsi qu'une plantation d'Eucalyptus au Brésil, puis utilisé pour modéliser le partitionnement de l'eau et de l'énergie à l'échelle de la parcelle pour le sol et la végétation. Une fois validée, cette version de MAESPA a été utilisée pour la fabrication de métamodèles pour les variables influencées par la complexité de la structure de la canopée, telles que l'extinction de la lumière, l'efficacité d'utilisation de la lumière, la transpiration ou la

température de canopée. Ces métamodèles ont ensuite été intégrés au nouveau modèle dynamique de culture pour lui permettre de simuler ces variables à l'échelle de l'arbre au lieu de l'échelle parcelle, et ainsi mieux prendre en compte l'anisotropie horizontale de ces variables. Ce modèle a ensuite été testé sur la plantation AFS de café d'Aquiaries au Costa Rica, et validé sur de nombreuses sorties dont les bilans de carbone, d'eau et d'énergie, ainsi que la production de café. Enfin, il a été utilisé pour prédire l'effet des changements climatiques sur deux sites d'altitude et de climat différents au Costa Rica, ainsi que pour étudier le potentiel d'adaptation de la culture de café par la gestion de l'ombrage. Les résultats des simulations montrent que ni l'effet d'augmentation de la photosynthèse par l'augmentation du CO<sub>2</sub> atmosphérique, ni les différentes gestions d'ombrage testées n'arrivent à compenser la réduction de la production de café dès lors que la température de l'air sort de la gamme optimale pour la plante (2020 à Aquiaries, 2060 à Tarrazu). Cependant, l'ajout d'ombrage au-dessus des caféiers permet de tamponner les pertes, et son effet est d'autant plus bénéfique lorsque le climat devient le moins adapté pour la production de café.

Il est évident que le modèle est encore récent et n'a donc pas été validé sur toutes les étapes phénologiques par manque de données, ni sur toutes les conditions climatiques sous lesquelles *C. arabica* est cultivé de nos jours. En effet, cette espèce est cultivée dans de nombreux pays sous des climats très différents qui influencent le développement des fruits. Par exemple la production de fruits en Colombie est pratiquement répartie sur toute l'année, alors qu'elle ne se fait qu'en une seule fois au Brésil ou en Ethiopie à cause de saisons plus marquées (Drinnan and Menzel, 1995). Il serait donc intéressant de tester notre modèle sur toute la gamme de conditions climatiques, pour voir s'il est capable de représenter ces différences de régime de floraison. De plus, parmi les dizaines (voire centaine) de gestions de l'ombrage possibles, seulement deux très contrastées (et leurs variantes) ont été testées aux côtés de la gestion en plein soleil. Il serait intéressant de tester des mélanges d'espèces plus complexes comme ceux rencontrés sur l'essai agroforestier du CATIE, avec des mélanges d'arbres taillés aux côtés d'arbres en croissance libre.

Le développement du modèle devra ensuite continuer pour intégrer d'autres processus tels que le cycle de l'azote, ou l'effet de l'ozone. Une fois plus complet, et validé sur plus de sites, le modèle pourrait aussi être utilisé comme outil de gestion.

Enfin, la méthodologie de couplage de modèles d'échelles différentes pourrait être utilisée pour simuler de nouvelles plantations pérennes et de systèmes agroforestiers grâce à l'utilisation d'autres modèles de croissance, et donc étudier l'effet des changements climatiques et de la gestion sur ces systèmes.





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# Annexe 1

## On the potential of agroforestry to buffer crop canopy temperature: a simple empirical model tested on coffee

Maxime Soma<sup>a,b,c</sup>, Rémi Vezy<sup>a,b,d</sup>, Lydie Guillion<sup>e</sup>, Gueric le Maire<sup>a,b,f</sup>, Elias de Melo Virginio Filho<sup>g</sup>, Karel Van den Meersche<sup>a,b,g</sup>, Jacques Avelino<sup>g,h</sup>, Olivier Roupsard<sup>a,b,g,\*</sup>.

<sup>a</sup>CIRAD, UMR Eco&Sols, F-34398 Montpellier, France

<sup>b</sup>Eco&Sols, Univ Montpellier, CIRAD, INRA, IRD, Montpellier SupAgro, Montpellier, France.

<sup>c</sup>INRA, UR 629, Ecologie des Forêts Méditerranéennes, Domaine Saint-Paul, 84917, Avignon, France

<sup>d</sup>INRA, UMR 1391 ISPA, F-33140 Villenave d'Ornon, France

<sup>e</sup>Montpellier SupAgro, département Biologie et Ecologie, bâtiment 18, 2 place Viala, 34060 Montpellier Cedex 02, France

<sup>f</sup>NIPE, University of Campinas, Campinas (SP), Brazil

<sup>g</sup>CATIE, Centro Agronómico Tropical de Investigación y Enseñanza, Turrialba 30501, Costa Rica

<sup>h</sup>CIRAD, UPR Bioagresseurs analyse et maîtrise du risque, F-34398 Montpellier, France

\**Corresponding author. Email address:* olivier.roupsard@cirad.fr (O. Roupsard)

### Abstract

Crop temperature, not air temperature, is the most relevant variable for adaptation to climate change, and generic agroforestry models are required to estimate it in a range of situations, from simple full sun (FS) to heterogeneous systems. Given the high complexity of the processes involved for estimating crop canopy temperature, we argue that empirical models built on experimental designs provide a reasonable alternative to process-based models. In a large and contrasted coffee agroforestry trial, we observed that FS coffee leaves can exceed air temperature by up to 5°C. High shading of coffees by agroforestry trees can pretend to reduce the maximum air temperature by 1.7°C and the coffee leaves temperature by 2.5°C compared to FS. A simple statistical model of generic purpose is proposed to estimate the coffee canopy temperature under shade trees ( $T_{Sh}$ ), using only air temperature ( $T_{air}$ ) and photosynthetically active radiation (PAR) variables from a weather station in full sun and canopy openness (CO) of shade trees. The RMSE obtained after cross-validation was 1.37°C, similar to current complex process models. Genericity of the model developed here to allows coffee canopy temperature mapping below any complex agroforestry system and estimations under future climate is discussed. Field evidences and modelling confirm that agroforestry is a relevant way for buffering the temperature increase due to future climate change, remaining fully compliant with other adaptation strategies.

**Keywords:** Coffee Agroforestry / Canopy openness / Crop Temperature / Adaptation / Model

**Abbreviations**

AIC: Akaike information criterion

ANOVA: Analysis of variance statistical test

C: *Chloroleucon eurycyclum* Barneby & J.W.Grimes

CO: Canopy openness (0-1 ratio)

DIFN: Diffuse non-interceptance (0-1 ratio)

□: difference shade-full sun for a given variable (Eq. 2)

E: *Erythrina poeppigiana* (Walp.) Cook

FS: full sun

FD<sub>PAR</sub>: Fraction of diffuse PAR (0-1)

GIS: Geographic information system

IC: Intensive conventional management

IO: Intensive organic management

LO: Low organic management

LAI: Leaf area index ( $m_{\text{leaf}}^2 m_{\text{soil}}^{-2}$ )

LAD: Leaf area density ( $m_{\text{leaf}}^2 m_{\text{crown}}^{-3}$ )

m.a.s.l.: meters above sea level (m)

PAR: Photosynthetically active radiation ( $\square \text{mol}_{\text{PAR}} \text{m}^{-2} \text{s}^{-1}$ )

Rh: Air relative humidity (%)

RMSE: Root mean squared error

Rn: net radiation ( $\text{W m}^{-2}$ )

ST: surface temperature (for use by remote sensors, °C)

T: *Terminalia amazonia* (J.F.Gmel.) Exell

T<sub>a</sub>: Air temperature (°C)

T<sub>a,max</sub>: Daily (24h) maximum air temperature (°C)

T<sub>a,min</sub>: Daily (24h) minimum air temperature (°C)

T<sub>c</sub>: Coffee canopy temperature (mean of 3 heights for T<sub>i</sub>, °C)

T<sub>i</sub>: Coffee leaf temperature measured by thermocouple (°C)

T<sub>r</sub>: Coffee crown radiometric temperature measured by thermoradiometers IR100 or IR120 (°C)

T<sub>s</sub>: Soil temperature measured by thermocouple (°C)

TukeyHSD: Tukey honest significance difference test

VHR: Very high resolution (image)

WS: Wind speed ( $\text{m s}^{-1}$ )

## 1. Introduction

As observed during the last 15 years, the stabilization trend and even the decline of yield in the major grain crops worldwide was attributed mainly to climate change and temperature issues (Brisson et al. (2010);(Ray et al., 2012)). Crop temperature is key to understand and model the variability of biological processes, such as phenophases, photosynthesis, transpiration, autotrophic and heterotrophic respiration. Air and crop temperatures in the field and their various forms (maximum, minimum, diurnal kinetics, etc.) present also serious challenges for crop sustainability through adaptation strategies (Way and Long, 2015). It is stressed here that the tropics are likely to have a shorter Time of Emergence (ToE), hence to be impacted sooner by the rapid phase of temperature increase (Hawkins and Sutton, 2012;Mahlstein et al., 2011) and stronger (Herold et al., 2017) than the temperate areas. However, the tropics benefit from a long-term experience in low-input and more resilient systems. In other words, the tropics provide a laboratory for the adaptation of agriculture in a changing climate.

Coffee is a tropical perennial crop grown in ca. 80 countries. Global coffee consumption is above 9 million tons, of which approximately 65% is from Arabica. Arabica originates from the forest understory of high plateaus in Eastern Africa, where air temperature is cool and shows little seasonal fluctuation. It is typically a mountain crop, requiring elevations between 800 and 2200 m.a.s.l, with an optimum range of temperature between 18 and 21°C (Alègre, 1959). Beyond 23°C, development and ripening of fruits are enhanced, but quality is affected, while relatively high temperature during blossoming, especially if associated to a prolonged dry season, may cause abortion of flowers (de Camargo, 1985). Continuous exposure to temperatures from 30 °C results in depressed and abnormal growth (Franco, 1958). According to suitability models, areas for Arabica were predicted to shrink, with ecological optima moving up to higher altitudes, and lower boundaries becoming unsuitable in the area of origin of Arabica (eastern Africa (Davis et al., 2012a;Moat et al., 2017)), but also in Mesoamerican lower altitude areas (Bunn et al., 2015;Ovalle-Rivera et al., 2015). Long-term options would be: (i) the relocation of Arabica to higher elevations, but only if land remains available (Baca et al., 2014); (ii) breeding coffee for adaptation to heat and drought stress, but this may take several decades before reaching effective results; (iii) grafting Arabica on Robusta (a lowland species, more heat and drought-tolerant), but this requires large investments and capacity building.

Alternatively, a short-term and readily available option to grow Arabica is through the proper management of shade trees in agroforestry systems, adjusting e.g. species, density, thinning and pruning according to elevation, exposure, and local microclimate. Agroforestry provides a bunch of ecosystem services (Meylan et al., 2017;Taugourdeau et al., 2014). It has been used since the beginning of plant domestication and sedentary agriculture (Mazoyer and Roudart, 2006), and is being revived also in temperate areas (den Herder et al., 2017). Agroforestry was already reported to be efficient in coffee systems for buffering temperature extremes during daytime, thereby avoiding temperature peaks and drastic drawbacks in net photosynthesis and fruit development (Barradas and Fanjul, 1986;Cannell, 1985a;DaMatta, 2004;Lin, 2007). However, air minimum

temperature ( $T_{a,min}$ ) was reported to be negatively correlated to coffee yield in Tanzania (Craparo et al., 2015b), and it should be more documented how agroforestry could increase  $T_{a,min}$ .

Given the high horizontal and vertical radiative heterogeneity occurring in agroforestry systems, and the number of processes involved it is generally considered of high complexity to simulate the foliage temperature in the understory through process based models (PBMs). Canopy and soil temperature ( $T_c$ ,  $T_s$ ) result from net incoming radiation (short and long waves) and energy fluxes (sensible heat flux and latent heat flux) balance (Cellier et al., 1993). PBMs explicitly represent the structure of the vegetation, the microclimate, the thermal properties of vegetation and soil, the radiative and energy fluxes (Bailey et al., 2016; Dauzat et al., 2001; Ngao et al., 2017). The key variable for the undercrop is the amount of transmitted global and thermal radiation by the shade trees, after considering the sun position, the fraction of diffuse light, the directional gap-fractions and after integrating in time, from the minute to the whole year. The canopy structure of shade trees (density, volume, porosity, projection, leaf area index and angles) has direct impact on light absorption by the coffee plants, as modelled by Charbonnier et al. (2013), and on its light-use efficiency (Charbonnier et al., 2017). Significant improvements on the estimation of canopy temperature ( $T_c$ ) of under-crops are thus expected from spatial integration of light availability, a first step required before modelling  $T_c$  with PBMs. Nevertheless, most PBMs still fail at describing important processes at the same resolution than radiation, such as turbulence and aerodynamic conductance. For instance, MAESPA (Duursma and Medlyn, 2012) uses the air temperature surrounding the crop to compute heat fluxes, but it is challenging to assess the spatial variability of surrounding air temperature.

Yet, we argue that there is no perfect tool to account for  $T_c$  in heterogeneous canopies, and that both empirical (Gaudio et al., 2017) and process-based approaches remain relevant and complementary. Here, we propose to empirically model the temperature of a coffee layer under spatially heterogeneous agroforestry system using only a reference standard weather-station in full sun and the canopy openness (CO) of shade trees. We used a long-term agroforestry trial (Haggar et al., 2011b; Schnabel et al., 2017), located at the lower elevation limit for Arabica cultivation, thus being representative for areas at threat under warming: this trial includes Shade x Management fixed factors, with numerous combinations, thus ideal to build the required database for such an empirical modelling approach. Although the relationships are valid mainly for coffee agroforestry, we consider that the method can be of generic relevance to address the complex problem of temperature in other understories, whatever the complexity of the upper-layer.

The aims of our study were:

- (i) to analyse the variability of coffee microclimate, soil and canopy temperature throughout a wide range of shade trees combinations permitted by an agroforestry trial, focusing on the effects of Shade and Management, of hour of the day, of height of measurement in the coffee canopy, of temperature measurements footprint (thermocouples, thermoradiometers and infrared cameras), of boundaries between plots;



- (ii) to propose a simple empirical model estimating the coffee canopy temperature, either for full sun ( $T_{c\_FS}$ ) or shade ( $T_{c\_Sh}$ ) conditions, and to discuss its genericity;
- (iii) to spatially interpolate and map coffee canopy temperature throughout a complex agroforestry design based on this model.

## 1. Material and methods

### 1.1. Site location and climate

The experiment was conducted in the coffee agroforestry trial Hagggar et al. (2011);(Schnabel et al., 2017) of CATIE (*Centro Agronómico Tropical de Investigación y Enseñanza*) in Turrialba, Costa Rica (9°53'46.0"N; 83°40'06.2"W), see Fig. 1. Elevation was 685 m.a.s.l. The mean annual temperature was 23°C, i.e. 2°C above the optimum range. We assumed there was no drought, considering a mean annual rainfall of 3200 mm with important precipitations throughout the year, even during the “drier” season (March-April) (Gómez-Delgado et al., 2011).

### 1.2. Experimental display

The experimental trial was set up in 2000 and studied continuously from 2015 to 2016. It is a 6-ha split-plot design comprising subplots (the replicates) of ca. 300 m<sup>2</sup> each (Fig. 1). Each subplot is one given combination of shade trees species (Shade, being the whole-plot factor) with various levels of fertilizers and pest management (Management being the split factor). For Shade, three species of shade trees are available alone or mixed, contrasting for phenology, shape, and use (Tab. 1): *Chloroleucon eurycyclum* (C), *Terminalia Amazonia* (T), *Erythrina poeppigiana* (E). At the time of our study, there were 645 shade trees all over the trial with specific densities. Full sun coffee plots with no shade trees were available as controls. Regarding Management, four treatments are available: Intensive (IC) and Medium (MC) conventional treatments, Intensive organic (IO) and low organic (LO) treatment, Intensive (IC) and medium (MC) conventional treatments followed the current methods for maximizing productivity, including pesticides and herbicides, while MC received half level of inputs. Intensive organic (IO) treatment includes manure and pesticides while low organic (LO) treatment only receives coffees and tree wastes and a manual weeding (more details in Hagggar et al., 2011). Each Shade x Management combination was replicated three times (3 blocks) and randomized. A total of 570 target coffee plants were measured for leaf temperature and microenvironment. Ten coffee plants per subplot were selected at different distances from the center, in such a way that they covered the whole plot: 10 coffee plants per subplot \* 19 sub-plots \* 3 blocks = 570 samples, mapped in Fig. 1. These plants were all in subplots inner rectangles of 300 m<sup>2</sup> to avoid border effects. These inner rectangles included around 150 coffee spots, planted at 2 x 1 m (planting density: 5000 holes ha<sup>-1</sup>, with 2 coffee plant stumps in each hole, pruned selectively every ca. 5-6 years).

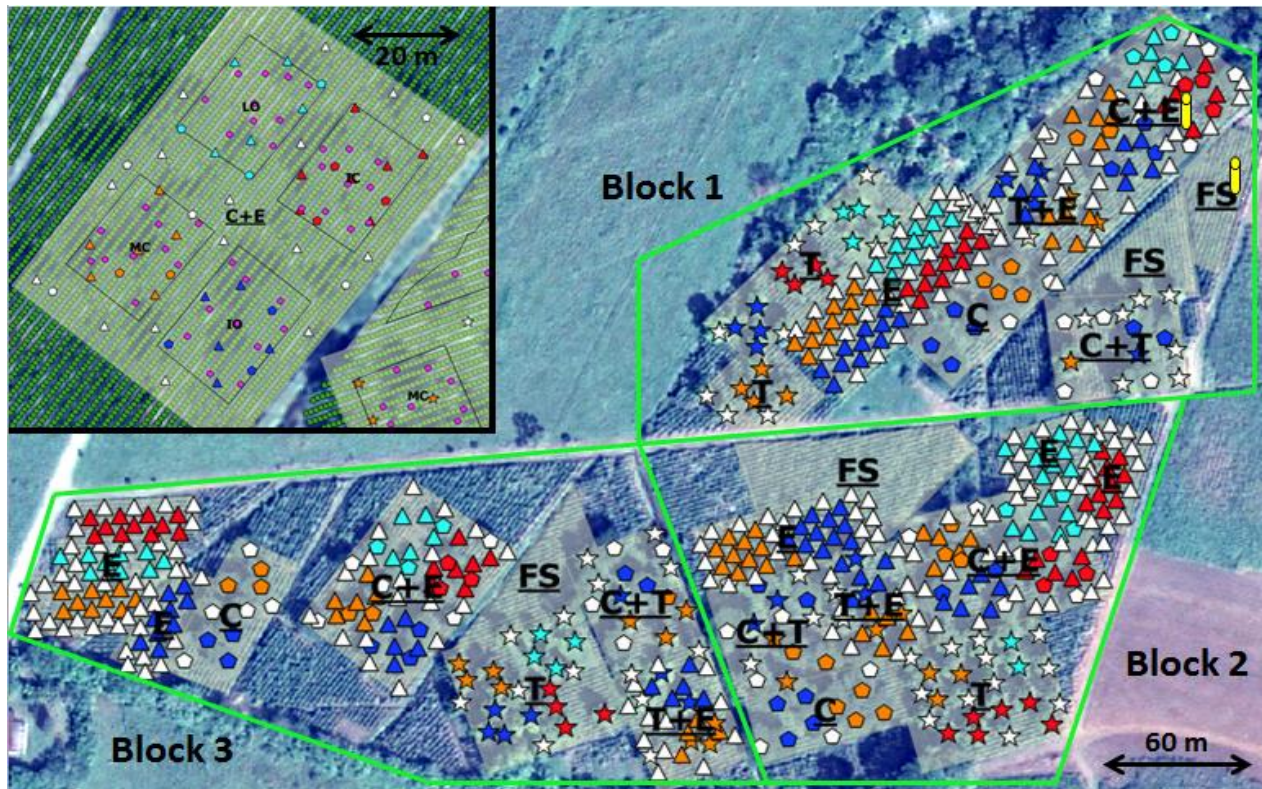


Figure 1: GIS map of the CATIE coffee agroforestry trial (6 ha). Green limits are for the three blocks. 645 shade trees' positions are displayed for the Shade factor (T = *Terminalia Amazonia* (★); C = *Chloroleucon eurycyclon* (○); E = *Erythrina poeppigiana* (△); FS = full sun). Tree color indicate Management (red: Intensive conventional (IC), orange: Medium conventional (MC), blue: Intensive organic (IO); sky blue: Low organic (LO) and white is for border trees). Yellow cylinders indicate the position of the reference full sun and shade microclimate antennas. The zip line was hanging in-between (not shown). The top-left insert is a zoom on C+E shade plot from block 1 (from top-right corner of main figure): all coffee plants appear as green dots; 4 Management subplots appear inside as black rectangles of 300 m<sup>2</sup> each, surrounded by borders; the randomly-selected target coffee plants for temperature measurements are displayed in pink.

Table 12: Shade tree species and coffee variety present in the CATIE agroforestry trial.

Species	Symbol	Phenology	Canopy shape	Use
<i>Chloroleucon eurycyclum</i> (Barneby & Grimes)	(C)	Defoliation March- April	High Spreading	Shade, high-value timber, N <sub>2</sub> -fixing
<i>Terminalia amazonia</i> (J.F. Gmel.)	(T)	Defoliation March- April	High compact	Shade, Timber
<i>Erythrina poeppigiana</i> (Walp.) O.F. Cook	(E)	Pollarded in February and August	Low compact	Shade, litter after pollarding, N <sub>2</sub> - fixing
<i>Coffea arabica</i> (L.) var. Caturra	-	Evergreen with seasonal variation <sup>a</sup>	Bush	Understory crop

<sup>a</sup>Coffee seasonal LAI variations reported in Taugourdeau et al. (2014)

### 1.3. Geographic Information System (GIS)

Two Very High Resolution images from the “Pleiades” satellite, (VHR: PAN (0.5m), R, G, B, NIR (2m)) were acquired in March and December 2013 (Le Maire et al., 2014) during the minimum and maximum coffee vegetation stages, respectively. Given the strong need for spatial referencing in this study, a GIS was created with the exact position of each shade tree and each of the 570 targeted coffees measured with a high-resolution GPS (Trimble Geo XT).

### 1.4. Shade tree inventory and canopy openness

An extensive shade tree survey (645 trees in total in the trial) was performed in September 2014 to record their location and size (tree and crown height, bole height, and diameter at breast height, DBH), using a 9-m pole, 2 orthogonal horizontal digital photographs and meter-tape. Tree height and crown height, width and horizontal projected area were computed after image re-scaling according to the pole. For each tree, we computed crown area on photos using the Google Sketchup™ free software. The crown volume was estimated using the mean radius and crown height.

Gap-fractions in the shade tree canopies were assessed by hemispherical photography, using a Nikon Coolpix 4500 camera mounted with a Nikon fisheye lens FC-E8 0.21x. All hemiphotos were taken vertically and upwards, from 20 cm above the 570 target coffee plants, under diffuse light conditions only to avoid specular reflections by foliage. We shot the photos during a stable shade tree phenological period of two months (14/04/2015 to 15/06/2015). Hemiphotos were analysed with the Gap Light Analyzer v2.0 software (GLA, (Frazer et al., 1999)), with visual threshold performed by one unique person, according to recommendations by Weiss et al. (2004). Each hemiphoto was divided into 36 azimuthal x 9 zenithal angles. Gap-fractions were computed using the “Gap Can Diffuse” output variable from GLA, *i.e.* the ratio of sky pixels to total pixels. Canopy openness (CO) varies between 0 and 1 and indicates the probability of diffuse radiation from the upper hemisphere to penetrate the canopy to a location. We used the DIFN method proposed in the Li-Cor LAI 2000 Plant Canopy Analyzer manual to compute canopy openness (Eq. 1):

$$CO = DIFN = \sum_{i=1}^9 GCD_i \cdot W_i' \quad \text{Eq. 1}$$

Where CO is the canopy openness, DIFN is the Diffuse Non-Interceptance,  $i$  is the number of the zenithal angle  $\theta$  (rad), GCD is the Gap Canopy Diffuse from GLA,  $W_i'$  is the normalized value of  $\sin \theta \cdot \cos \theta \cdot d\theta$  and  $d\theta$  is the angle interval (rad).

We computed  $W_i'$  for the 9 zenithal angles of the hemiphotos, following the method proposed for 5 angles in the LAI 2000, resulting in the following [angle;  $W_i'$ ] couples: [5-0.030]; [15-0.087]; [25-0.133]; [35-0.163]; [45-0.174]; [55-0.163]; [65-0.133]; [75-0.087]; [85-0.030].

## 1.5. Microclimate

### 1.5.1. Micro-dataloggers for $T_a$ in agroforestry plots

We studied the semi-hourly variability of  $T_a$  (including night and day minimal, mean, and maximal temperatures) in a few selected agroforestry and full sun plots using micro-dataloggers placed in home-made white plastic ventilated shelters. In subplots of interest, 4 iButtons (model DS1922L-F5#, Thermochron, Embedded Data Systems), were settled to monitor air temperature at 1 m above ground. This experiment lasted for 1.5 month (13/05/2015 to 23/06/2015).

### 1.5.2. Reference static weather stations on 2 antennas in full sun and shade plots.

Microclimate measurements took place during one full year, from 15/03/2015 to 14/03/2016. Two reference automatic weather-stations were settled on 2 antennas separated by 40 m (Fig. 1). The first antenna (10 m high) was located in a full sun (FS) coffee plot and the second one (30 m high) in the nearby dense *Chloroleucum\*Erythrina* (C+E) shade plot (Sh, Block 1, FS and C+E, Fig. 1).

Each antenna was equipped with a data-logger (CR1000, Campbell Scientific) and monitored the following data every 30 sec, then averaged every 1 min and every 30 min: air temperature ( $T_a$ ) + air humidity (Rh) measured at 2 m high (just above the coffee canopy) by CS215 (Campbell Scientific) in ventilated shelter; soil thermocouples (TFCC/TFCP-020-100, Omega Eng., Inc.) mounted in opposite series and connected to multiplexor (AM16/32B, Campbell Scientific) monitored soil temperature differences at 0, -2, -5, -15, -30, -60, -100 and -150 cm underground with an additional absolute reference temperature at -2 m; soil humidity measured at -15, -30, -60 and -90 cm (CS615, Campbell Scientific) with a second multiplexor.

In addition, the full sun reference antenna was equipped with a Photosynthetic Active Radiation ( $PAR_{FS}$ ) sensor (Li-190sb, Li-Cor), a net radiation sensor ( $Rn_{FS}$ , NR-Lite, Kipp & Zonen), a wind sentry ( $WS_{FS}$  WindSonic 2D, Campbell scientific) and a pluviometer ( $Rain_{FS}$ , TE525mm, Campbell Scientific). The fraction of diffuse PAR ( $FD_{PAR,FS}$ ) was computed following the model proposed by Spitters et al. (1986).

### 1.5.3. Coffee leaf ( $T_l$ ), canopy ( $T_c$ ) and radiative ( $T_{r\_IR100}$ , $T_{r\_IR120}$ , Thermal image) temperatures

Three coffee plants were chosen randomly nearby each reference antenna and for each of them, 3 thin copper-constantan thermocouples (TFCC/TFCP-005, Omega) were attached with medical permeable tape to the lower (abaxial) side of the leaf lamina, with the tip slightly inserted into the leaf tissue. Mature leaves, nearby the end of the branches were selected at low, middle, and top height of the coffee canopy, in order to monitor leaf temperature ( $T_l$ ) at 3 coffee canopy heights, with their average ( $T_c$ ). We checked the quality of the thermocouple contact with the leaf every week, and re-located it when necessary. We assumed a footprint of ca. 1 mm<sup>2</sup> for each thermocouple.

A narrow-range (half angle view of 5°) thermoradiometer (IR100, Campbell Scientific) was fixed 50 cm above one of the coffee plants' crown for each antenna, directed downwards to monitor the top-canopy

radiative temperature ( $T_{r\_IR100}$ ), in the centre of the crown, i.e. around the upper leaf thermocouple ( $T_{l,high}$ ). We assumed a constant emissivity of 0.98 (López et al., 2012) and a footprint of around 60 cm<sup>2</sup> for  $T_{r\_IR100}$ . In order to allow future extrapolation to the surface temperature (ST) that can be remotely-sensed, a wide-range (half angle view of 20°) thermoradiometer (IR120, Campbell Scientific) was fixed at 10 m on each antenna, pointing downwards at 30° from vertical, towards the 3 coffee plants gauged with thermocouples. It is assumed that the footprint of  $T_{r\_IR120}$  was ca. 40 m<sup>2</sup>, including profiles into coffee plant canopies and soil portions. Both thermoradiometers were sheltered and used the body temperature as a reference for surface temperature.

Thermal images were acquired with a Fluke Ti400 thermal imager, including a 320 x 240 pixels sensor, 1.31 mRad resolution, accuracy  $\pm 2^\circ\text{C}$ , thermal sensitivity  $\leq 0.05^\circ\text{C}$ . We shot the coffee plants from the FS antenna towards the 4 cardinal azimuths and drew temperature transects between row (coffee canopy top) and interrow (soil).

#### **1.5.4. Mobile weather stations on pole and zip line**

A mobile weather station was equipped to sample the 570 target coffee plants, similarly to the ones under reference antennas, using a 3 m-high pole with tripod, with air temperature and humidity sensors, anemometer, PAR sensor, two thermocouples for soil temperature (row and between coffee row, just below the soil surface), and three thermocouples for coffee  $T_1$  and  $T_c$ . The mobile antenna was moved in every Shade x Management plots, to the 570 target coffee plants (Fig. 1). Measurements lasted two months (from 14/04/2015 to 15/06/2015), the pole was randomly moved every day intra-plots and inter-plots by blocks and, at the end of the period, 10 coffees plants have been measured in each subplot.

In order to study border effects, i.e. thermal transitions between adjacent full sun and shade plots, a zip line was settled between FS and C+E antennas, perpendicular to the coffee rows (Fig. 1). A hanging Campbell datalogger was displaced along the 40-m zip line equipped with labels every 2 meter, measuring  $T_{r\_IR100}$  above the coffee layer every minute. Thirty-five transects were performed during 12 sunny days of July and August 2015, each one lasting around 15 min. We used the  $T_{r\_IR100}$  value obtained close to the FS antenna as a reference for every single  $T_{r\_IR100}$  point of each transect.

#### **1.5.5. Sensor inter-calibration**

We performed sensor inter-calibration in a ventilated greenhouse for 4 days, prior to displaying them in the field, namely PAR sensors, temperature + humidity sensors, and iButtons. For temperature and humidity, our references were respectively a copper-constantan thermocouple and brand new CS215 (Campbell scientific). All iButtons were hanged together in a ventilated net and in the shade for several days. Temperature probes and thermocouples were placed at few centimetres from iButtons. Several inter-calibration curves were fitted, especially for the iButtons and applied prior to comparing readings.

In the field, we compared the mobile pole and the full sun reference antenna, leaving the mobile pole exactly at the same place for 5 days (15-19 of June 2015), with its thermocouples positioned close to the reference, and recording every minute. We successfully checked that all TC gave very consistent results. We also checked for the other sensors, and re-calibrated whenever necessary (data not shown). The pole data were stored every min, its datalogger was synchronized with the ones of antennas every day.

### **1.5.6. Absolute and differential ( $\Delta$ ) measurement modes**

The micrometeorological and temperature variables (*Var*) were analysed either in absolute or in differential mode. In differential mode, we computed the difference ( $\Delta$ ) between the shade and reference full sun measurements, both recorded at the same period (1 or 30 min or 24h), as the following:

$$\Delta Var = Var_{_Sh} - Var_{_FS}. \quad \text{Eq. 2}$$

With *Var*, the variable of interest; subscripts *\_Sh*= shade (agroforestry); *\_FS* = reference in full sun.

## **1.6. Statistical analysis**

All database management and analysis were performed in R open software (R Core Team, 2015).

### **1.6.1. Method of contrasts**

The CATIE coffee agroforestry split-plot trial (Fig. 1) displayed 7 Shade types (whole-plot factor) and 4 Management levels (subplot-factor), replicated into 3 blocks (SUPPL. MAT. I). However, it was imbalanced, in the sense that it excluded a few non-viable Management levels in the Shade types. For example, full sun plots came only with IC and MC, because organic management would collapse there (SUPPL. MAT. I); pure stands of the N-fixing tree *Chloroleucum* were only managed with MC and IO. Hence, we relied on the method of contrasts to guarantee statistical balance: we repeated statistical tests per Shade groups that shared the same Management levels (more details in Hagggar et al. (2011)).

### **1.6.2. Fixed effect of Shade on plot air temperature (iButtons data)**

Analysis was performed in 3 contrasted treatments: full sun (FS), *Erythrina* (E), and *Chloroleucum* + *Erythrina* (C+E). Parametric tests for the Shade fixed effect were performed through ANOVA and TukeyHSD (“stats” package, “anova” and “TukeyHSD” functions).

### **1.6.3. Fixed effect of Shade on coffee canopy temperature and microenvironment (mobile weather station data)**

The medium conventional (MC) Management level was the only one common to all Shade types (SUPPL. MAT. I). We therefore applied ANOVA and TukeyHSD tests on MC plots to compare Shade types.

#### 1.6.4. Geostatistics

We applied semi-variograms and kriging (“gstat” package, “fit.variogram” and “krige” functions) to interpolate tree canopy openness and  $T_c$  between measurement points. Assumption of normality and heterogeneous spatial repartition (absence of continuous trend through the whole trial) were checked (“gstat” package, “variograms” function). Accuracy was assessed through cross validations and Pearson’s moment correlation coefficient (“stats” package, “cor.test” function).

#### 1.6.5. Multivariate modelling for the estimation of coffee canopy temperature ( $T_c$ )

Measurements made in the full sun reference static weather station provided a large temporal dataset of  $T_{c\_FS}$  and  $T_{r\_IR100}$  that could be used for modelling coffee canopy temperature in full sun. Indeed, the more data, the more accurate and generic can be empirical models because it encompasses more environmental and physiological conditions. In the other hand, the mobile weather station provided a rich database of  $T_{c\_Sh}$  under various shade trees species, densities, and management. Each model was computed following the same modelling approach:

- Since many variables were measured in this experiment, a feature selection was made in two steps to minimize overfitting while keeping model performance and genericity (Saeys et al., 2007). First, only variables classically measured in standard meteorological stations, and with good precision, were chosen as predictive variables in order to keep the model applicable elsewhere. For example, soil surface temperature would have been a good predictor, but was not kept in the model because not commonly measured in meteorological stations, and highly variable in space. Then, six automatic features selection were used to rank their importance. The algorithms being used were: the recursive feature selection, stepwise, Random Forest, bootstrapped relative importance, MARS and Boruta. The mean rank of each variable using the different algorithms was computed, and only the variables with the highest overall score were kept for use in each model.
- A model selection was made using a repeated k-fold cross-validation (10 folds repeated 5 times) to build the best model out of the previously selected variables, and to check for the coefficients and goodness-of-fit variability. The resubstitution error (i.e. in-sample error) is computed from this step because it gives information on the error that the model makes while modelling the data. It represents the variance that the model cannot explain by itself.
- A “two-deep” cross-validation (Jonathan et al., 2000) was performed by applying the model only once to a validation set of data to assess the generalization error using the out-of-sample RMSE. This step is important because the validation set is the only sample that is truly independent on the model building, and is the only way to assess the model prediction accuracy and genericity.

## 2. Results

### 2.1. Microclimate from Full sun and Shade antennas

Time series of daily rainfall and net radiation as measured with the reference full sun antenna were presented in Fig. 2a,b for one entire year (06/03/2015 to 05/03/2016). There was no marked dry season (Fig. 2a). Although  $T_a$  and VPD appeared only marginally lower in the shade plot (Fig. 2c,d), by less than 1°C and 1hPa, respectively, soil temperature was markedly lower (by up to 1 °C at 200 cm and up to 3°C at 2 cm deep, Fig. 2e), confirming an important microclimate effect induced by Shade.

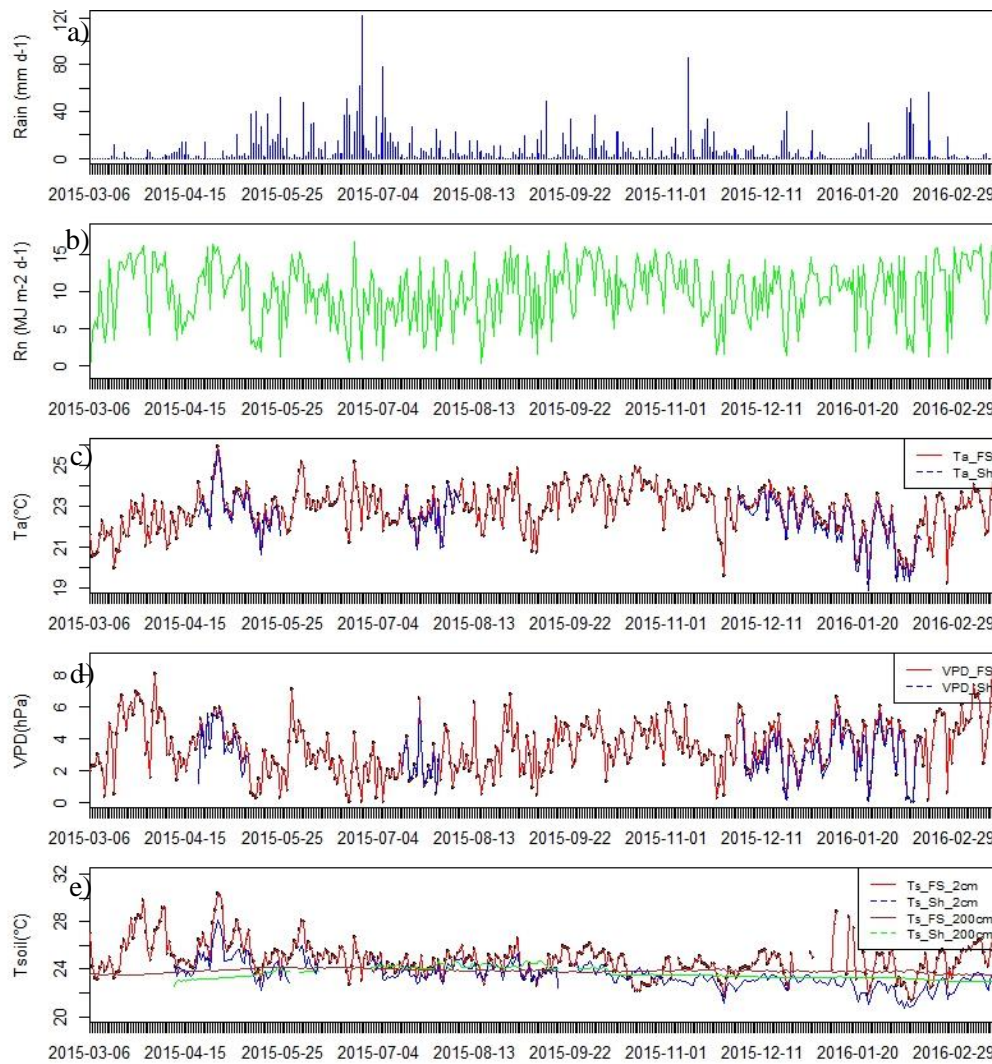
**Table 13: Survey of shade tree sizes in the coffee agroforestry trial, measured 14 years after planting.**

Shade tree	Tree height (m)	DBH (cm)	Crown height (m)	Crown width (m)	Crown volume (m <sup>3</sup> )
<i>Chloroleucon eurycyclum</i>	18.7 <i>a</i> (2.2)	145.5 <i>a</i> (17.1)	11.8 <i>a</i> (2.1)	13.7 <i>a</i> (2.4)	9688 <i>a</i> (4102)
<i>Terminalia amazonia</i>	17.9 <i>a</i> (3.4)	110.6 <i>b</i> (23.2)	11.8 <i>a</i> (3.4)	9.5 <i>b</i> (2.6)	5260 <i>b</i> (3338)
<i>Erythrina poepiggiana</i> (pollarded)	4.64 <i>b</i> (1.8)	98.1 <i>c</i> (37.5)	2.6 <i>b</i> (1.2)	3.7 <i>c</i> (1.7)	232 <i>c</i> (270)

NB: Letters account for TukeyHSD significant difference between species. Values in brackets are standard deviations.

DBH: diameter at breast height. N= 645 trees surveyed.

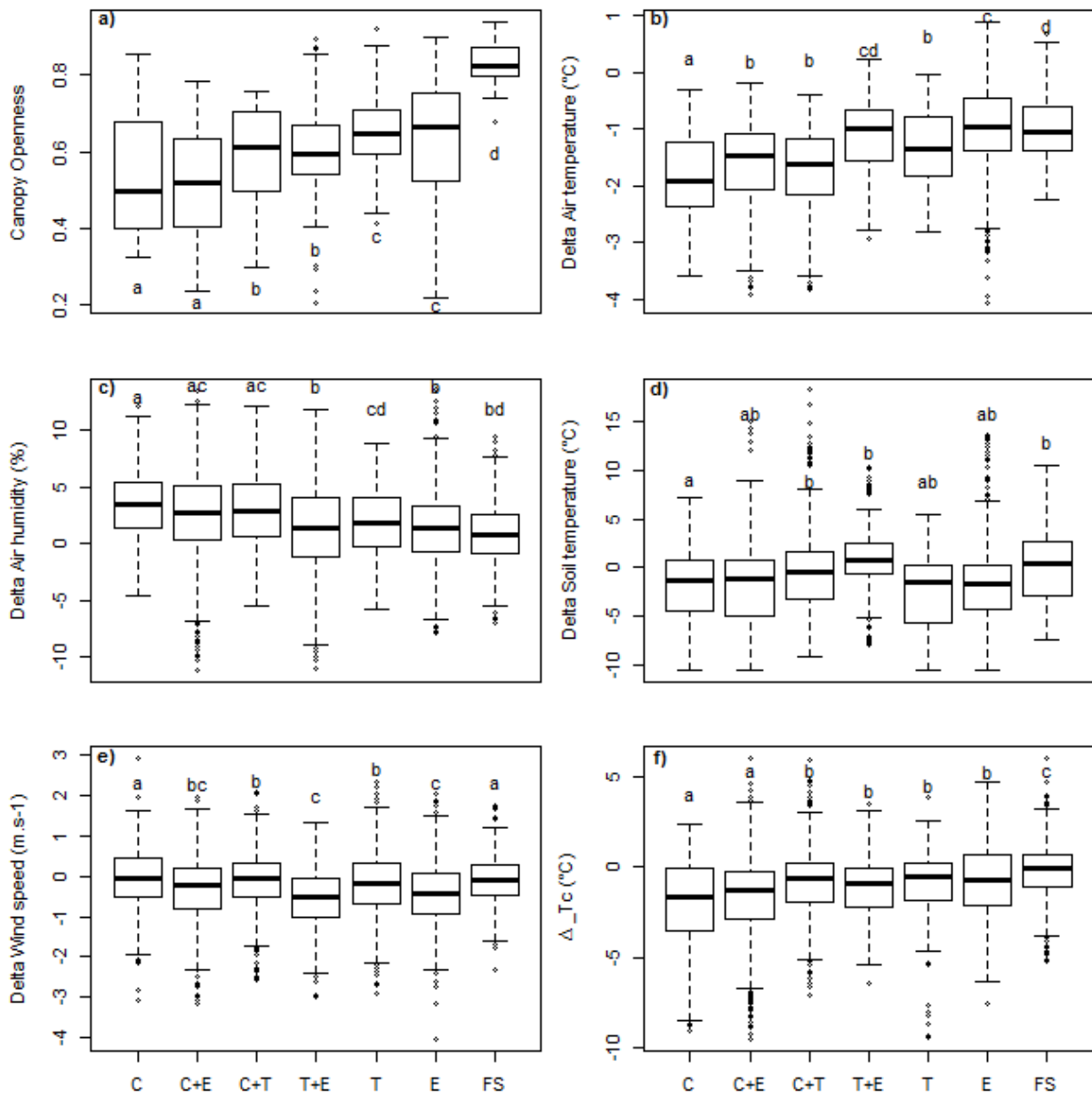




**Figure 2:** Daily microclimate in CATIE agroforestry trial, compared between full sun (FS) and shade (Sh) reference antennas for one-year (06/03/2015 to 05/03/2016): a) Rainfall (FS); b) Net radiation (FS); c) Air temperature, compared; d) VPD, compared; e) Soil temperature at 0 and 200 cm deep, compared. Missing data for  $T_a$  and VPD under shade were due to instrument breakdowns. One dot is the daily average (or sum for Rain and Rn) of 48 semi-hours.

## 2.2. Shade tree survey

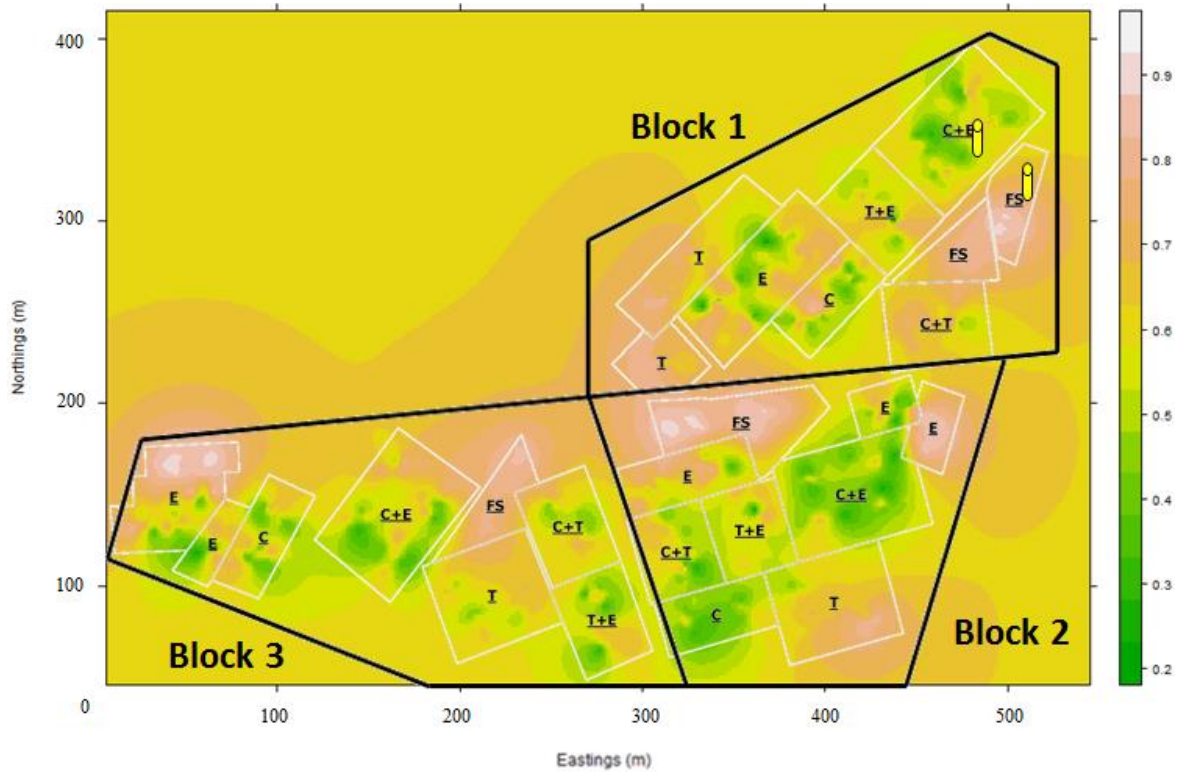
We encountered significant differences in shade tree (*Chloroleucon* (C), *Terminalia* (T) and *Erythrina* (E)) size variables, excepted for tree height and crown height in C and T (Table 2). C and T were much taller trees with wide crowns when compared to E, a consequence of the pollarding of E every year. Although C and T reached the same height and crown height, C expressed larger bole diameter at breast height, crown width and crown volume. C and C+E expressed the lowest tree canopy openness (CO), i.e. the largest Shade effect (Fig. 3a), second came C+T and T+E, third T and E and fourth, as expected, FS. This indicated that our 2 antennas represented the extreme conditions for shade in this trial. In FS, canopy CO was  $< 1$ , due to the influence of edges in neighboring plots. Consistently, we encountered higher canopy openness in the center of the FS plots, up to a maximum of 0.95 (data not shown). The variability of CO was minimum in FS and maximum in E, likely due to small E crowns distributed in plots.



**Figure 3: Shade trees canopy openness and effects on coffee microclimate.** a) Shade canopy openness (CO): CO was ranked in increasing order from left to right sides and the same order was adopted for the next plots. In full sun, CO remained less than 1 due to the neighboring plots; N = 570 hemiphotos taken 20 cm above each target coffee plants; b) to e) Differences in diurnal microclimate variables ( $\Delta\_Var$ ), measured with a mobile pole and computed between Shade types and full sun, following Eq. 2. All measurements compared at the same minute. Only results of MC Management were presented here for simplicity; N = 210 measurements (10 coffees \* 7 subplots \* 3 blocks); f) Differences in leaf temperature ( $\Delta\_Tc$ ). N = 201 measurements; C= Chloroleucon; T = Terminalia; E = Erythrina. Letters account for significant difference (Tukey pairwise test, p-value < 0.05). o are outlier values, dotted low and dotted high vertical lines extent respectively to smallest value and highest value (outliers excluded), solid low and solid high horizontal lines are respectively at lower and upper quartiles, middle bold line is median value.

Using the 570 hemiphotos, we built a CO kriged map with a one-meter resolution after kriging (details in *SUPPL. MAT. II*). Full sun plots are easily identifiable in Fig. 4, with highest and homogeneous level of transmitted light (1 to 0.8, white and pink colors) except close to boundaries with agroforestry plots. C and C+E plots displayed the lowest CO values (green color). However, situations in other intermediate treatments

were more difficult to distinguish. The map revealed a large intra-plot variability as well, highlighting the presence of numerous gaps between shade trees, with consequences on the variability of dependent variables, such as the amount of light transmitted and the leaf temperature.



**Figure 4:** Kriged map of shade tree canopy openness (CO) in the CATIE agroforestry trial. Grey lines represent the borders of the whole-plot treatment (Shade factor) and black lines are for the 3 blocks. C = *Chloroleucon*; T = *Terminalia*; E = *Erythrina*; Cylinders symbols are for reference weather stations (blue: shaded in C+E, red: in full sun, FS). N = 570 canopy openness measurements used for kriging.

## 2.3. Coffee microclimate

### 2.3.1. Effects of Shade on air temperature

Shade reduced diurnal maximum air temperature ( $T_{a,max}$ ) measured with iButtons by around  $1.7^{\circ}\text{C}$  under C+E stands, when compared to FS (Table 13). In E pure stand, only a slight but non-significant trend to buffer  $T_{a,max}$  was observed as compared to FS. The daily average air temperature ( $T_a$ ) values were significantly reduced under shade, by  $0.5^{\circ}\text{C}$  when comparing C+E with FS, or by  $0.19^{\circ}\text{C}$  when comparing C+E with E. No significant Shade effect was detected for  $T_{a,min}$ , indicating negligible effect of tree cover at night.

**Table 3: Differences of air temperature ( $T_a$ ) between plots. Four iButtons microdataloggers by Shade were settled in each Management plot 1 m aboveground; (\*\*\*) : very highly significant difference ( $p < 0.001$ ); (\*\*): highly significant difference ( $p < 0.01$ ); (\*): significant difference ( $p < 0.05$ ); NS: non-significant difference. N=1995 half-hourly observations for each sensor monitored from 13/05/2015 to 23/06/2015.**

Shade effect	TukeyHSD difference (p-value)		
	Mean daily $T_a$	Daily $T_{a,min}$	Daily $T_{a,max}$
(C+E) - E	- 0.3 (***)	0.18 (NS)	- 1.34 (**)
(C+E) - FS	- 0.5 (***)	0.15 (NS)	- 1.71 (***)
E - FS	- 0.19 (**)	- 0.04 (NS)	- 0.37 (NS)

### 2.3.2. Effects of Shade and Management on coffee microclimate

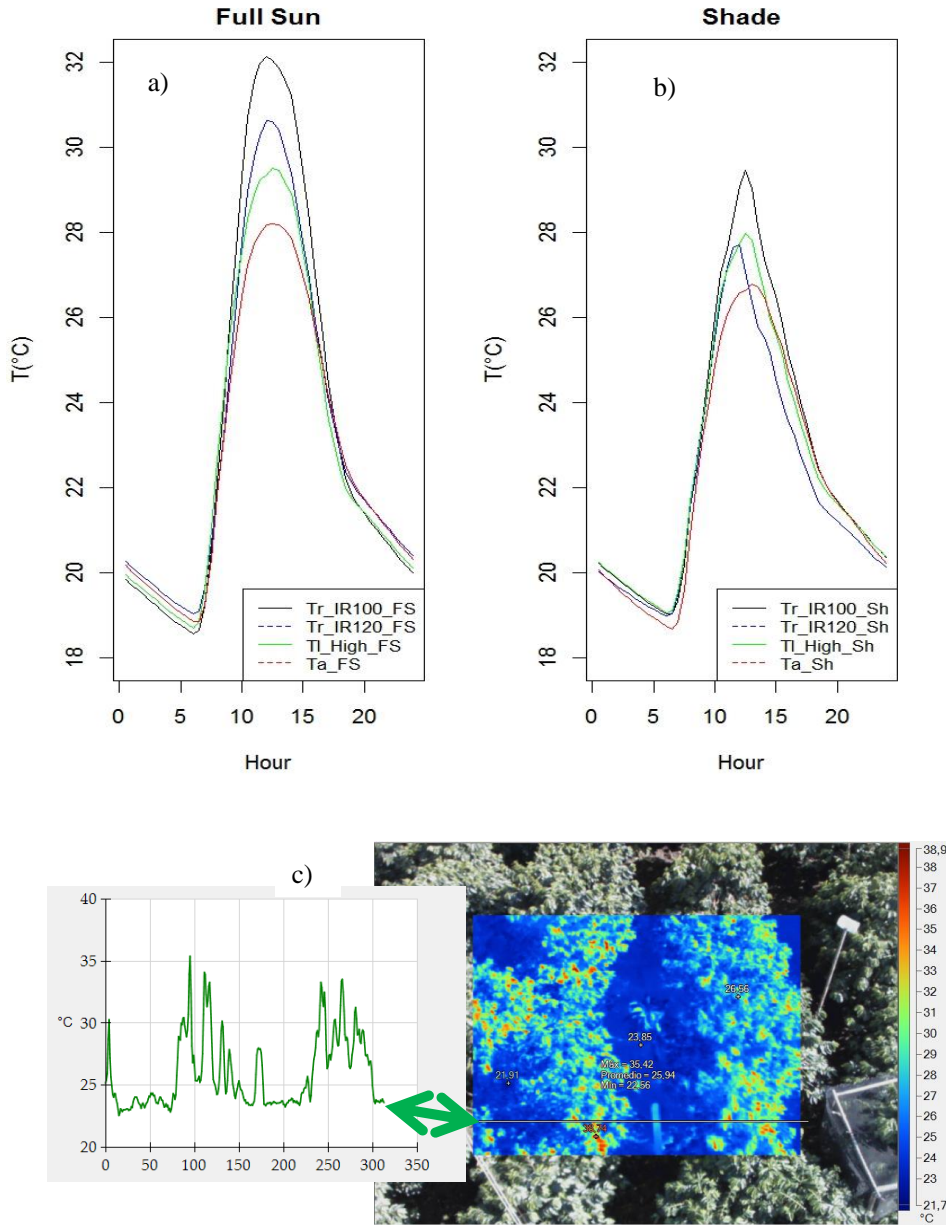
The pole measurements occurred diurnally only, and confirmed the results from the iButton 24h approach for  $T_a$ . The Shade effect was very highly significant on all computed  $\Delta$  according to Eq. 2, but the Management effect was globally much less significant (data not shown). Given the prevalence of the Shade effect, and for the sake of simplicity, we pursued the analysis only on Medium conventional (MC) management level that was available for every Shade type (Fig. 3b to e).  $T_a$  was progressively cooling when canopy openness decreased (Fig. 3b) down to  $-1.7^\circ\text{C}$  for the C treatment. It should be stressed that even mobile pole measurements in the full sun treatment expressed lower  $\Delta T_a$  values than reference full sun weather station: indeed, some coffee measurements with the pole were close to borders, thus were influenced by the shade of edge agroforestry treatments.  $\Delta Rh$  had significantly higher air humidity under shade (Fig. 3c), by up to 3%. Soil temperature ( $\Delta T_s$ , Fig. 3d) diminished under shade, with about the same magnitude and a much larger variability than for  $\Delta T_a$ . Windspeed differences ( $\Delta WS$ ) appeared more disconnected from the canopy openness gradient but could be reduced by  $0.5 \text{ m s}^{-1}$  under E treatments only (Fig. 3e): E in pure or in mixed (T+E, C+E) stands induced significantly reduced wind speed, possibly a consequence of the low height of E, whereas taller trees (C and T) had little influence on WS. Noteworthy, higher air temperatures were observed in shade plots including tall trees and E (C+E and T+E) than in pure C and T stands (Fig. 3b), which could possibly be a consequence of reduced wind speed under the low canopy of E.

## 2.4. Variability of coffee leaf and canopy temperatures

### 2.4.1. Footprint of the thermal sensors

We used one year of 30 min data in FS (Fig. 5a, left panel) to compare the daily time-courses of  $T_a$ ,  $T_{L,High}$  (leaf temperature at the top of coffee canopy),  $T_{r,IR100}$  (radiative temperature from the IR100 directed to the crown centre), and  $T_{r,IR120}$  (radiative temperature from the IR120 directed to a large spot of coffee crowns and soil). All sensors expressed similar values during the night-time, confirming consistency between the various temperature measurement methods. However, for diurnal periods, the various sensors expressed large discrepancies: the overall ranking was  $T_{r,IR100} > T_{r,IR120} > T_{L,High} > T_c > T_a$ .  $T_{r,IR120}$  could be  $3^\circ\text{C}$  higher than  $T_{L,High}$ . As  $T_{r,IR100}$  could be up to  $2^\circ\text{C}$  higher than  $T_{r,IR120}$  as measured with similar techniques, the top canopy

was likely warmer than the whole canopy seen with a 30° angle from vertical. Indeed,  $T_{L\_High}$  was to the most 2°C higher than  $T_c$ , indicating that coffee canopy temperature decreases downwards the canopy.  $T_{r\_IR100}$  could be up to 5°C higher than  $T_{L\_High}$  in FS (Fig. 5a, left panel). Whether or not the top crown centre (where  $T_{r\_IR100}$  is pointed) could be much warmer than the top crown edge (where  $T_{L\_High}$  is positioned) was checked further using thermal imaging (Fig. 5b).



**Figure 5: Variability of temperature readings.** Daily time-course of temperatures measured on the full sun (FS) reference antenna:  $T_a$  (air temperature),  $T_{L\_High}$  (the average of 3 upper leaves on three coffee plants measured by thermocouple),  $T_{r\_IR100}$  (radiative temperature from the IR100 directed in the crown center, above  $T_l$  of plant 1),  $T_{r\_IR120}$  (radiative temperature from the IR120 directed to a large spot of coffee crowns at 30° angle from vertical). All data from full sun reference antenna, at 30 min time-step (2015-2016); Idem for the reference shade antenna. Thermal image showing large thermal gradients between row and interrow. Image taken on 14/10/2015 at 08h01 AM,  $T_{min} = 21.91^\circ\text{C}$  (interrow);  $T_{max} = 38.74^\circ\text{C}$  (leaves from canopy top). The white line indicates the position of transect.

Temperature transects of these thermal images confirmed large variations perpendicular to the row, with up to 10°C more around the crown centre than in the crown borders and interrow, and with a large micro-local

variability. In the shade reference (Fig. 5a, right panel), the maxima of  $T_{r\_IR100}$  and  $T_{r\_IR120}$  were lower than in full sun (Fig. 5a, left panel), by around 2.5 °C, which is much more than  $T_a$  differences, which remained below 1.7°C. Comparing the shape of the curves, we found no particular spreading of the afternoon cooling under shade.

### 2.4.2. Coffee crown temperature profiles

We compared the diurnal leaf temperature ( $T_l$ ) measured by thermocouple, first between full sun (FS) and C+E shade situations (i.e. the densest shade), and also between coffee crown levels (high, medium and low) (Table ). For diurnal periods, shade trees systematically reduced coffee leaf temperature, whatever the crown level. This Shade effect was more pronounced in the lower part of the canopy (by around -1.14°C) than in the highest part (by around -0.51°C only). In the C+E shade plot, the lower part of the crown was significantly and gradually cooler than the top crown (-0.54°C) , but there was hardly any such effect in FS.

**Table 4: Differences of average coffee leaf diurnal temperature ( $T_l$ ) measured by thermocouple between full sun (FS) and shade (C+E) plots (grey cells), or between 3 crown levels in the same plot (Low, Middle, High, white cells). The difference was always computed as the coolest minus the warmest, as follows:  $VAR_{Sh} - VAR_{FS}$  and  $VAR_{Lower\ Crown} - VAR_{High\ Crown}$ . Negative values indicate a cooling effect.**

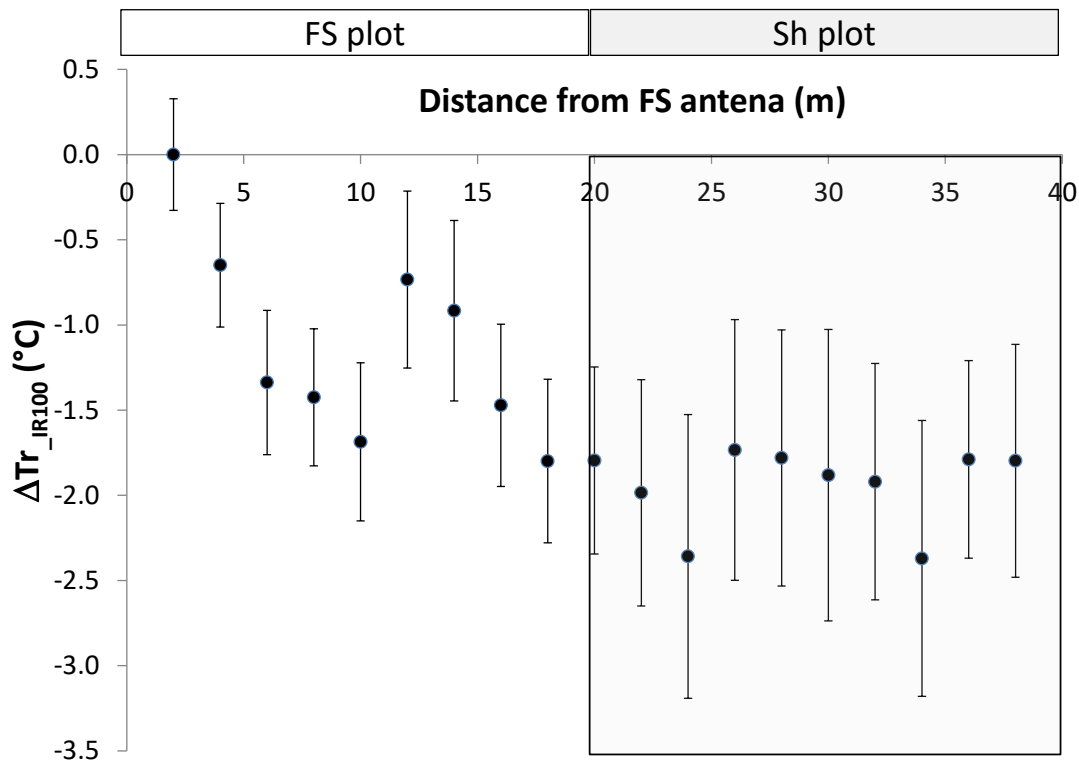
Tukey HSD difference		Full sun reference station			Shade C+E reference station		
		Low	Middle	High	Low	Middle	High
<b>Full sun reference station</b>	Low						
	Middle	-0.07(NS)					
	High	-0.18*	-0.1NS				
<b>C+E reference station</b>	Low	-1.14***	-1.2***	-1.32***			
	Middle	-0.87***	-0.94***	-1.05***	-0.27**		
	High	-0.33***	-0.40***	-0.51***	-0.82***	-0.54***	

In the following, we assume that averaging  $T_l$  over the 3 FS plants and over 3 canopy heights (9 sensors averaged) is a reasonable proxy for the reference FS coffee canopy temperature ( $T_{c\_FS}$ ), while  $T_{l\_High\_FS}$  (the average of 3 upper leaves from 3 coffee plants) is a proxy for the FS coffee top canopy.

### 2.4.3. Border effects between plots: zip line between FS and C+E

We obtained rather stable values for  $Tr_{IR100}$  under the C+E shaded plot, all around 2°C below the reference value obtained in the middle of the FS plot (Fig. 6). The transition to the FS plot was progressive and quite linear along the 20 m that separated the FS plot edge from the FS antenna located in the middle of the FS plot (Fig. 1), indicating that shade trees have long-distance border effects on the microclimate.





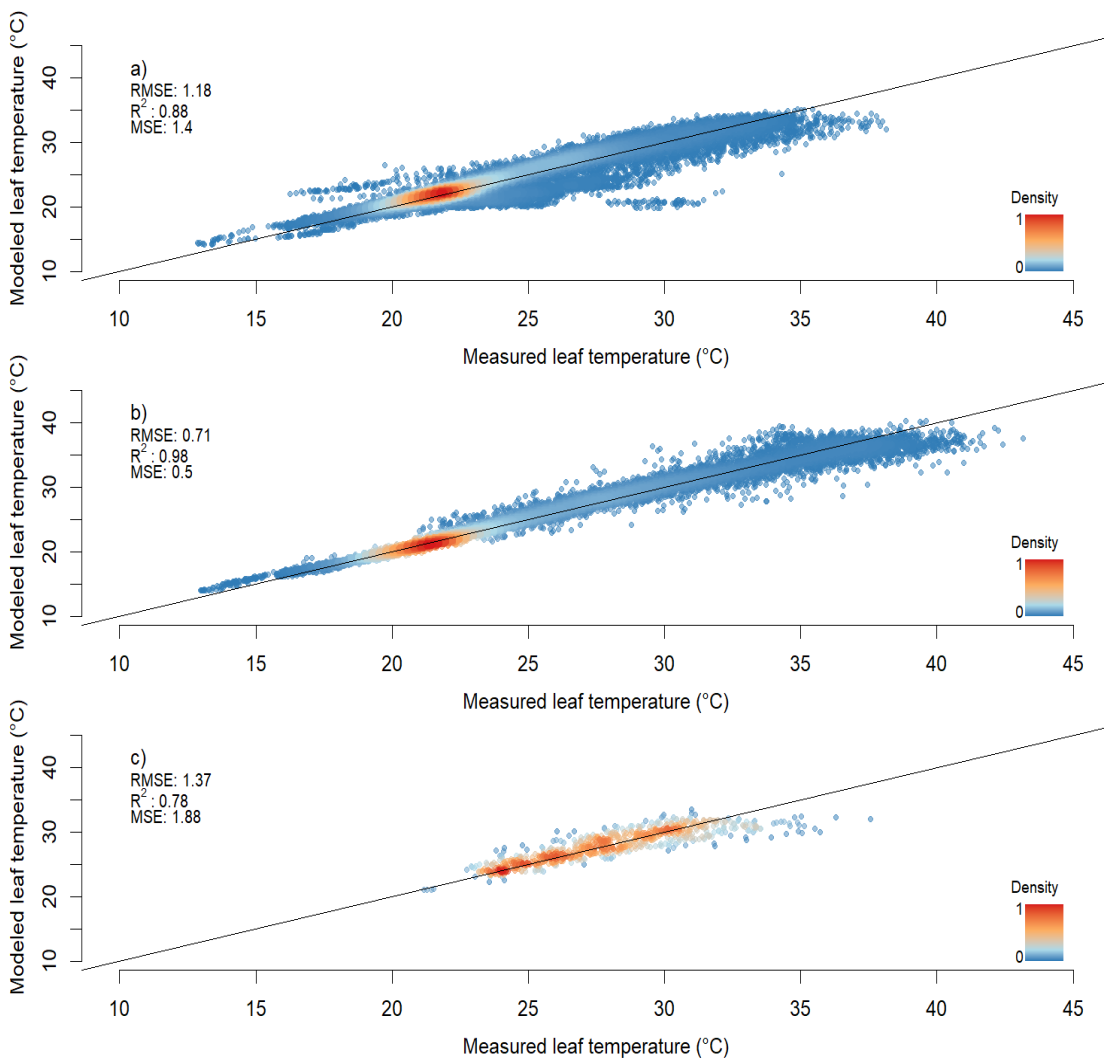
**Figure 6: Border effects:  $\Delta Tr_{IR100}$  (Eq. 2) transition between shade C+E and full sun plots, obtained along a 40 m long zip line. Each dot is the average of 35 points measured every 2 m during 12 shiny days on the zip line transect, above the coffee layer. Error bars are SE.**

## 2.5. Empirical model of $T_c$

### 2.5.1. Empirical model for $T_{c\_FS}$

The coffee canopy temperature ranged from 13°C to 39°C for  $T_{c\_FS}$  and 13°C to 44°C for  $T_{r\_IR100}$  in the whole data set (Fig. 7a,b). Hence, two different models are proposed, using either  $T_{c\_FS}$  or  $T_{r\_IR100}$ . Both models used the same three predictors for FS: air temperature ( $T_{a\_FS}$ ), PAR ( $PAR_{FS}$ ) and  $Rh_{FS}$  (Table 5). The model that was fitted using  $T_{r\_IR100}$  presented both lower in and out-sample error, and far less outliers (Figure 7 a,b). The repeated k-fold cross-validation showed a low variance in RMSE for both models, and low variance in coefficients estimations (not shown). Surprisingly, out-sample RMSE were lower than in-sample error, but giving the large dataset on which the models were fitted, it is possible that some outlier values with low leverage were present during fitting, but absent from the validation set.

Model accuracy was 1.18°C and 0.71°C (RMSE) for  $T_{c\_FS}$  and  $T_{r\_IR100}$  respectively, which appeared relatively low considering the wide range of monitored values and several months of implementation.



**Figure 7: Measured and modeled coffee canopy temperature: a) in full sun using thermocouples ( $T_c$ ); b) in full sun using IR100; c) in agroforestry system using thermocouples ( $T_c$ ). One dot is one-minute measurement from the cross-validation set only. Colors indicate point density. Black line is identity function.**

### 2.5.2. Empirical model for $T_{c\_Sh}$

Coffee  $T_c$ , as measured diurnally only using a mobile weather station, ranged from 21°C to 37.5°C (Fig. 7c). The best predictor variables were found to be  $T_{a\_FS}$ ,  $PAR_{FS}$ , and  $CO_{FS}$ . We also tested the fraction of diffuse PAR in the model, but it did not bring improvement. All model parameters are given in Table 5. Although RMSE was higher than for the two previous models, Figure 7c shows that its predictions were quite in agreement with the measurements.



**Table 5: Multiple regression models for coffee canopy temperature in full sun (FS) or shade (Sh) situations. N= 127800 observations (80% test/train; 20% validation). In-sample RMSE standard deviation comes from the repeated k-fold cross-validation (CV).**

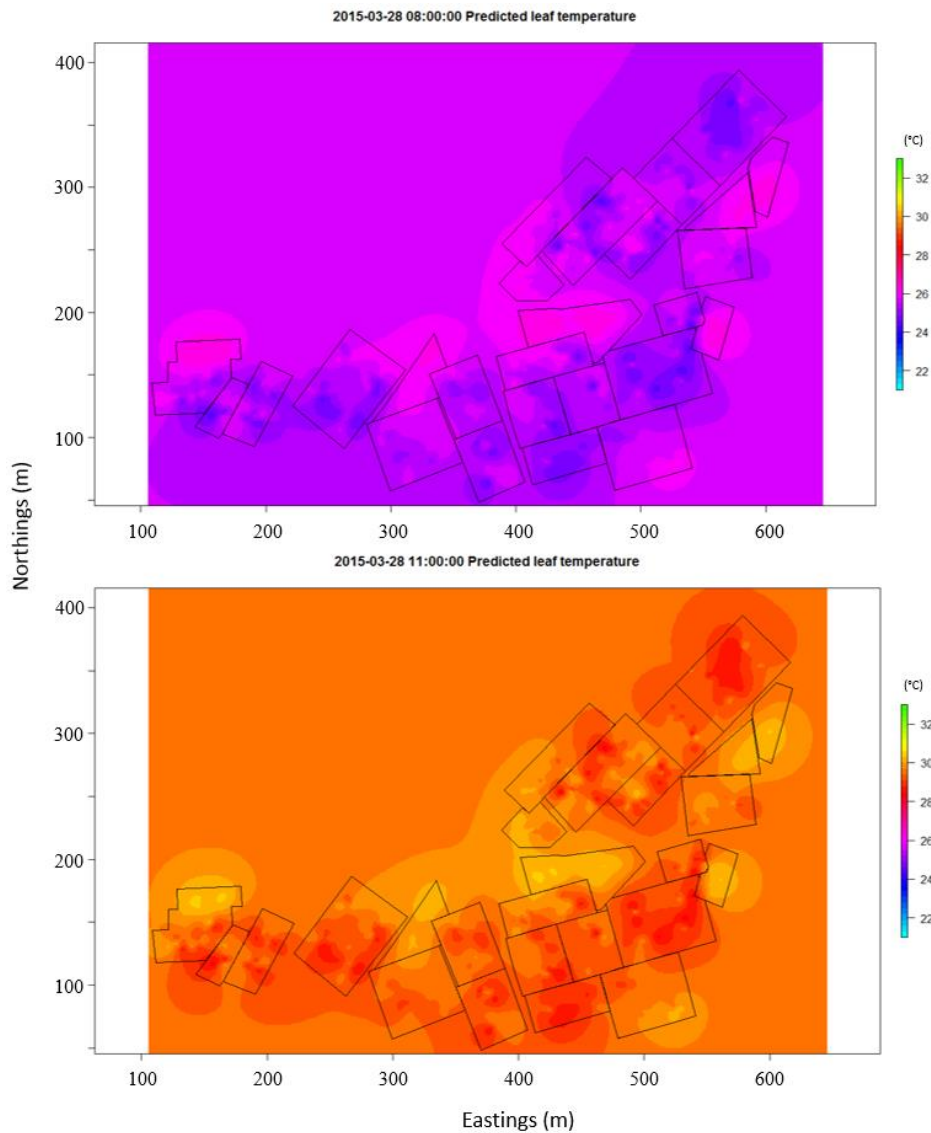
Model type	Variable	Unit	Estimate	Standard error	p-value	In-sample RMSE (SD)	Out-sample RMSE
<b>T<sub>c</sub>_FS</b>	Intercept	Celsius	-2.486	0.145	<0.0001***	1.36°C (0.02)	1.18°C
	Ta_FS	Celsius	0.944	$3.15 \cdot 10^{-3}$	<0.0001***		
	PAR_FS	$\mu\text{mol m}^{-2} \text{s}^{-1}$	$1.96 \cdot 10^{-3}$	$1.75 \cdot 10^{-5}$	<0.0001***		
	Rh_FS	%	$4.01 \cdot 10^{-2}$	$9.53 \cdot 10^{-4}$	<0.0001***		
<b>T<sub>r</sub>_IR100_</b> FS	Intercept	Celsius	6.0176	$8.48 \cdot 10^{-2}$	<0.0001***	0.80°C (0.01)	0.71°C
	Ta_FS	Celsius	0.872	$1.85 \cdot 10^{-3}$	<0.0001***		
	PAR_FS	$\mu\text{mol m}^{-2} \text{s}^{-1}$	$3.40 \cdot 10^{-3}$	$1.03 \cdot 10^{-5}$	<0.0001***		
	Rh_FS	%	$3.85 \cdot 10^{-2}$	$5.59 \cdot 10^{-4}$	<0.0001***		
<b>T<sub>c</sub>_Sh</b>	Intercept	Celsius	1.381	$4.53 \cdot 10^{-1}$	$2.32 \cdot 10^{-3}$	1.39°C (0.05)	1.37°C
	Ta_FS	Celsius	$8.34 \cdot 10^{-1}$	$1.80 \cdot 10^{-2}$	<0.0001***		
	PAR_FS	$\mu\text{mol m}^{-2} \text{s}^{-1}$	$9.58 \cdot 10^{-4}$	$7.20 \cdot 10^{-5}$	<0.0001***		
	CO_Sh	%	3.197	$1.59 \cdot 10^{-1}$	<0.0001***		

## 2.6. Mapping coffee canopy temperature (T<sub>c</sub>) for the whole trial

We used the T<sub>c,Sh</sub> empirical model to predict T<sub>c,mod</sub> for any condition of time, light or shade. Kriged maps of predicted coffee canopy temperature (T<sub>c,mod</sub>) are presented according to the hour of the day (Fig. 8). In the morning (8AM, Fig. 8a), T<sub>c,FS</sub> was on average predicted 2° C higher than under highly shaded conditions. Overall, large intra-plot variability and border effects were observed, in accordance with previous results. Around noon (Fig. 8b) an average reduction of 3.2°C was observed between full sun and highly shaded plots (C/C+E).

## 3. Discussion

Our main hypothesis here was that agroforestry could damp the temperature extremes of the undercrop by the same order of magnitude than expected from the temperature increase under future climate change. We proposed to verify this assert in a mature, large and complex agroforestry trial, combining Shade (different species and densities of shade trees) and Management (4 levels of inputs) levels.



**Figure 8:** Kriged map of predicted coffee canopy temperature ( $T_{c,mod}$ ) by the empirical model. Example on 2015-03-28 at 8h00 AM (top) and 11h00 AM (bottom). Temperatures in °C. N=570 kriged values. Color scale in °C.

### 3.1. Comparing instrumentation for assessing canopy temperature. Footprint considerations.

Leaf temperature measurement in its natural environment is considered difficult (Bailey et al., 2016; López et al., 2012; Ziegler-Jöns et al., 1986). Agreements between methods are usually good at night or on shade leaves, provided that the emissivity is correct. However, for leaves in direct sunlight, several degrees of difference have been reported between thermocouples (warmer) and thermographic cameras (Bailey et al., 2016), with the maximum thermocouple measurement error during sunlight hours around 3°C, and less than 1°C at night, while the RMSE was 2.1°C.

Considering our very similar values observed at night-time when temperature gradients are minimal in the plot, and large thermal gradients revealed by temperature transects perpendicular to the coffee row (thermal

images), we argue here that diurnal differences between thermoradiometers and thermocouples are most likely due to spatial variability and footprint issues, not to instrumentation bias or calibration issues. Indeed, the footprint of leaf thermocouple is in  $\text{mm}^2$ , whereas thermoradiometers integrate over several  $\text{dm}^2$  or  $\text{m}^2$ , even possibly including soil patches in the case of IR120 at  $30^\circ$  angle. Consequently, the meaning of “canopy temperature” is likely more dependent on the spatial variability and on footprint than on instrumentation. When the desired footprint is superior or equal to the  $\text{m}^2$ , it is much unlikely that thermocouples would provide a faithful canopy temperature reading, given its extreme local variability (up to  $10^\circ\text{C}$  measured by IR camera between soil and top crown). In such case, we recommend using thermoradiometers.

An outcome of canopy temperature studies as provided here would be also the verification of land surface temperature (LST) products retrieved from thermal infrared (TIR) remote sensing data, e.g. the use of the thermal bands of the Moderate Resolution Imaging Spectrometer (MODIS) onboard the Terra and Aqua satellite, the thermal band of the Thematic Mapper (TM) onboard the LANDSAT-5 platform or Enhanced Thematic Mapper (ETM+) onboard the LANDSAT-7 platform (Sobrino et al., 2004;Sobrino et al., 2008), or of surface energy balance models (Bastiaanssen et al., 1998). Broad-view thermoradiometers (such as IR120 measuring from top of antenna here) do provide a more adequate ground-truth reference for such remotely-sensed products.

### **3.2. Can agroforestry substantially buffer microclimate and crop canopy temperature?**

Regarding coffee leaf temperature in full sun conditions, we found an average midday difference of  $+5^\circ\text{C}$  between coffee maximum leaf and maximum air temperature, and no difference for night minimal temperature (Fig. 5a), which confirmed previous studies (Lin, 2007;López-Bravo et al., 2012;Siles et al., 2010). Such differences tended to vanish at low solar elevation and were nil at night. Cotton leaves were found cooler or equal to air temperature (Lu et al., 1994). This large midday difference in  $T_{l,\text{max}}$  observed here in coffee is likely a consequence of low stomatal conductance around noon, as often reported in the coffee photosynthesis literature (DaMatta et al., 2007;Franck et al., 2006).

Air temperature became gradually cooler following denser shade. We found buffered air temperature in shaded plot C+E (as compared to the FS reference weather station) by  $-0.5^\circ\text{C}$  for mean daily temperature ( $T_a$ ), no significant effect for  $T_{a,\text{min}}$  and  $-1.71^\circ\text{C}$  for  $T_{a,\text{max}}$  (Table 3). IR100 showed coffee canopy cooling effects under shade by up to  $2.5^\circ\text{C}$  (Fig. 5b), which is around  $1^\circ\text{C}$  more than for air temperature. Therefore, the shade effect is enhanced when considering the canopy temperature, instead of the air temperature only. The relative humidity was higher in shaded plots. A reduced vapour pressure deficit in shaded plots is expected to favour stomatal opening, a critical aspect in the coffee leaf physiology. Many studies demonstrated a strong limitation of photosynthesis in leaves of *Coffea arabica* to diffusive factors, together with a strong stomatal sensitivity to VPD (Batista et al., 2012;Martins et al., 2014). However, higher humidity and frequency of leaf wetness favour coffee leaf rust (*Hemileia vastatrix*), especially when the fruit load is high (López-Bravo et al., 2012). Soil temperature was sampled across the agroforestry trial and confirmed the  $T_a$  results. Wind speed

differences were driven by the presence of *Erythrina* (E). We can reasonably assume that given the low height of this pollarded tree, the aerodynamic resistance was increased closer to the coffee canopy. Consistently, we observed higher temperature in C+E and T+E than in pure C and T plus higher temperature in E than in FS. Optional agroforestry systems leave the trees in plot borders as windbreaks. Although not being studied here, windbreaks could impact on crop temperature according to local reduction or increase of turbulence (Thofelt et al., 1984).

Overall, coffee can express large (up to 5°C) differences of canopy temperature with respect to the surrounding air, when observed in the full sun. High shading (C or C+E) can pretend to reduce daily  $T_{\text{air,max}}$  by -1.7°C. Now considering daily mean values on leaves, the reduction would be only by -0.5 to -1.1 °C, depending on the coffee crown level (Table 4). We confirm that shade is a reasonable option to consider for partially mitigating the effects of temperature rise due to climate changes predicted for the end of the century. The benefit of shade appears higher when considering  $T_{\text{max}}$  than for  $T_{\text{mean}}$ , and when considering canopy temperature rather than air temperature.

### **3.3. Does agroforestry also affect $T_{\text{a,min}}$ ?**

As a component of the well-documented buffering effect of the shade tree canopy on daily temperature,  $T_{\text{a,min}}$  has also often been reported to increase under shade trees in other ecosystems (Ferrez et al., 2011;Gaudio et al., 2017;Morecroft et al., 1998), depending greatly on LAI (von Arx et al., 2012). A recent study (Craparo et al., 2015) underlined a negative statistical correlation between daily  $T_{\text{a,min}}$  (which is generally obtained during the night-time) and yield of Arabica coffee at the scale of Tanzania. This correlation is noteworthy, although being mainly statistical. Our results did not confirm Craparo et al. (2015), we found no significant difference between air  $T_{\text{a,min}}$  in agroforestry plots or in full sun situations. Lin (2007) obtained less than 1°C difference as well. Caramori et al. (1996) found much higher minimal temperature under shade tree, ranging +2 to +4°C, i.e. one order of magnitude more than in our study, but their location was much cooler, including frost periods. Hence, it is possible that for very different range of temperatures (less than 10°C) shade trees could buffer minimal temperature and provide frost protection. Depending on the main tree species, the buffering effect can be higher for  $T_{\text{min}}$  or  $T_{\text{max}}$ , due to differences in canopy closure (Renaud and Rebetez, 2009). Gaudio et al. (2017) reported that, due to thermal inertia and lower wind below shade, T remains higher than expected under shade in the late afternoon, while air cools faster in full sun, but we did not observe any specific curve cooling spreading in the afternoon here (Fig. 5b).

### **3.4. Does Management have an important effect on coffee canopy temperature?**

The effects of fertilizing and controlling pests chemically, or not, was found relatively negligible on air and coffee canopy temperature, as compared to the shade effect, or even not detected. It also means that coffee microclimate was not modified due to Management, and probably that gaps in shade tree cover were equally distributed without much influence of fertilization level on tree foliage. However, pruning events on *Erythrina*

were more intensive in IC and IO sub-treatments to provide more or less organic inputs from branches. Here we developed our relationships in a period devoid of pollarding, but pollarding and tree thinning could further affect coffee canopy temperature more abruptly.

### **3.5. Intra and inter-plot variability of canopy openness and temperature in agroforestry systems and trials**

Although Shade played a major role for explaining differences of temperature, large intra-plot variability was observed. Such variance was likely due to numerous gaps between shade trees, in particular regarding small sized trees like *Erythrina* (e.g. very intense shading under the tree and almost full sun situations a few meters aside). However, it should be noted that the intra-plot variability was also enhanced by the presence of dissimilar plots with contrasting structure beyond the borders. Borders tend to exaggerate the inherent intra-plot variability, thus to reduce the level of significance of the statistical effects. Considering the variability encountered even in the full sun treatment due to borders, with a plot canopy openness of 0.8 instead of being 1, a  $\Delta_{T_{air}}$  of 1.1°C instead of being nil, and a linear relationship between  $\Delta T_r$  and the distance to FS plot edge for more than 20 m (Fig. 6), it is argued that much larger plots with negligible border effects would probably have magnified the Shade effects on microclimate, first because the FS plots would not have been cooled by lateral shaded plots and second because shade plots in contact with full sun plots would have been cooler. Nevertheless, despite temperature effects probably attenuated by the border effects, most Shade effects remained significant in our trial.

### **3.6. Advantages of using the continuous variable “Canopy openness” rather than the commonly used “Shade” fixed effect**

In such a context of large intra-plot variability, fixed factors such as Shade or Shade species have little significance at the coffee plant scale, as already pointed out by Charbonnier et al. (2013), who mapped the high intra-plot heterogeneity of light availability and absorption by the coffee layer in agroforestry conditions. Canopy openness is a quantity varying between 0 and 1 indicating the probability of diffuse radiation from the upper hemisphere to penetrate the canopy to a particular location. It reflects the structure above the point independently of the amount, the direction (zenithal and azimuthal) and of the nature (direct or diffuse) of light. It can be measured in many points of the plot and mapped. Large gaps revealed in shaded plots here (Fig. 4) point out the limits of studies using shade treatments as fixed effects, especially when the plot size is too small. We obtained higher scores with models using the continuous variable canopy openness instead of the fixed variable Shade, demonstrating the benefit of preferring continuous variables rather than fixed effects. Moreover, a sparse tree canopy structure (e.g. *Erythrina*) was proved to be a source of errors in heat fluxes models due to strong horizontal and vertical heterogeneity (Kustas and Norman, 1999) which could be partly resolved with a finer description of the intra-plot variability of light transmittance. Canopy openness is generic and it can be rapidly assessed with hemiphotos (Gaudio et al., 2017) or even by densitometers (Lemmon, 1956). In our study, one measurement every 30 m<sup>2</sup> appeared to be sufficient, but it would be worth checking

how much this distance could be extended. Although not proposed here, hemiphotos also offer the possibility to draw the relationship between canopy gaps and zenithal or azimuthal angles. Combined with Leaf Area Density, Leaf Angle Distribution, phenology, sun position, light intensity and fraction of diffuse light, this information permits to compute light availability above the coffee plant, the first step to compute its absorbed light, for periods from the semi hour to the entire year, using various kinds of light transfer models (Bailey et al., 2016;Charbonnier et al., 2013;Dauzat et al., 2001).

### **3.7. A simple model to infer coffee canopy temperature from the structure of shade trees in agroforestry systems**

We aimed to build a simple (empirical and using easily accessible parameters) and as generic as possible (for coffee system, from full sun to agroforestry, whatever the shade tree species) model to spatially extrapolate our results and provide quantitative estimations for farmers and stakeholders in management strategies.

The  $T_c$  model requires only  $T_{a,FS}$ ,  $PAR_{FS}$ , and the canopy openness (CO), i.e. only measurements from a standard weather station which could be outside of the plantations and hemiphotos, or densitometer or Licor LAI-2000, if available. The strong influence of the fraction of diffuse light, a consequence of cloudy conditions, was pointed out by several heat fluxes and organ temperature measurements (Guilioni et al., 2000;Lhomme and Guilioni, 2004;Morillas et al., 2014). However, although we attempted to introduce the fraction of diffuse light into our empirical model here, it did not improve the overall predictions and we discarded it.

In terms of model accuracy (RMSE), it should be stressed that we opted for a mobile pole, going through very numerous conditions (570 observations in 19 treatments and in 3 blocks). We discarded the option to install a large number of antennas in several treatments for obvious financial reasons and also security of the equipment. Hence, the  $T_c$  model proposed here was assumed reliable on average, with its RMSE of 1.37°C, obtained after cross-validation. Using a refined 3D ray-tracing model, Bailey et al. (2016b) reported RMSE varying from 1.4 to 1.9 °C, which is in the same order of magnitude than our estimates using a much simpler model here. Many other temperature models showed similarly high RMSE values, including detailed ones (~1.5°C (Guilioni et al., 2000) in maize) and in particular when dealing with extreme values (3.5°C in (Lhomme and Guilioni, 2004)). Similar difficulties were experienced for instantaneous measurements in heat fluxes by Morillas et al. (2014), resolved by daily value measurement instead of minute scale.

We could not measure at night in the numerous Shade treatments for security reason. However,  $T_{min,Shade}$  was not different from  $T_{min,FS}$  and  $T_{r,night}$  was not very different from  $T_{air,night}$ : therefore, we argue that  $T_{c,night}$  can reasonably be estimated by  $T_{air,night}$ . Consequently, the model performed reasonably in a very large set of conditions.

Coffee canopy absolute temperature of the full sun reference can be approximated too, with a slightly better performance when using the  $T_{c,FS}$  model. We observed that full sun coffee canopy temperature could be computed easily with air temperature, PAR and air humidity. This model is in accordance with other organ scale models which were found mostly dependent on air temperature (Guilioni et al., 2000). Conformity is

also observed in more complex upscale heat fluxes models where air temperature is considered as input but not solar elevation or air humidity (Norman et al., 1995; Baldocchi et al., 2000). More precise models for absolute organ temperatures were developed with complex and numerous inputs but remained hardly applicable outside research purposes due to their complexity (Guilioni and Lhomme, 2006).

Overall, with air temperature, PAR, air humidity and canopy openness, a reasonable approximation of coffee canopy temperature can be proposed whatever the shade in agroforestry systems. Another application of such a simple model is for ground estimations, as required in remotely sensed applications (Sobrino et al., 2004; Sobrino et al., 2008), or for the detection of surface temperature, sensible and latent heat fluxes for instance (Bastiaanssen et al., 1998).

Nevertheless, the model should still be used with caution on coffee crops under water stress, or on others undercrops that might have some very different rates of transpiration, or in highly turbulent conditions (close to windbreaks for instance). A verification/recalibration step is recommended on such situations and offers some room for further experimentation. However, we assume that the model should remain quite reliable whatever the elevation, a prevalent parameter to consider normally in coffee cropping, considering that it already incorporates the temperature of the surrounding air mass.

### **3.8. Trade-off between canopy temperature, light availability, drought and yield in a warmer climate**

It was often reported that when coffee is cultivated in optimal conditions, shade reduced its yield (DaMatta, 2004), and that intensification using chemical solutions against pests sustained coffee yield. This has led to large intensification of coffee production, wherever the farmers could afford these inputs despite the fluctuations of the market price. In opposite conditions, agroforestry remained popular in suboptimal conditions (Muschler, 2001). We stress here that high temperatures jeopardize the full sun intensive system. And this perspective is even worse under dry conditions. Hence, global solutions must be applied to allow perpetuation of this crop with its inherent economic and social implications. In absence of any adaptation measures, the current area occupied by Arabica coffee could be converted either into Robusta coffee, or, e.g. cacao. Three levels of solution can be distinguished. The first one is, as experienced here, through modifying the structure of the tree canopy above the crop: here we tested the effect of Shade and concluded that it was effective in regulating  $T_{\max}$  and  $T_{\text{mean}}$ , whereas it had little effect on  $T_{\min}$ , and least in non-frosting conditions. One advantage of agroforestry is that it is a readily available solution, already implemented and proven in the past for its resilience to e.g. economic difficulties, when the price of coffee is low, and inputs have to be minimized. Most adaptation options build on existing practices and sustainable agriculture, rather than new technologies (Jarvis et al., 2011). Some more technical and long-term solution relies on breeding and F1 hybridization (Bertrand et al., 2011) and grafting on Robusta root systems through biotechnologies. Such methods gather a lot of support (Way and Long, 2015). However, applications of these researches are still to come and require time-consuming verifications with poorly known consequences. A crucial point is the capital necessary to adopt such intensified and technological options, especially for small farmers who are

often not able to purchase seeds and accompanying inputs with high risk of bankruptcy. All the above-mentioned solutions should allow maintaining the coffee activities in their current area under future climate changes. Last solution is through re-locations at higher altitude, implying hard competition with others agricultural activities, such as pasture, sugar-cane etc.: this solution is purely impossible to apply if higher altitudes are not available as it is the case in many countries cultivating Arabica. Our study and others (Lin, 2007b) confirm that agroforestry has to be considered a major solution, in particular for its short-term capacity of implementation, additional incomes from wood products with respect to yield and constitute a cheaper option for farmers. Fortunately, agroforestry gains to be combined with other options (breeding, hybridization, grafting). In addition, shade tree cover is a flexible component of the environment crops as it can be more or less dense, in space or in time. Simple models such as proposed here were meant to ease the shade management.

#### **4. Conclusions**

The forecasted increase of temperature, and by extension changes in other plant environment as humidity and soil properties, are predicted to seriously affect production and even sustainability of major crops and farming systems. It is up to stakeholders and farmers to decide what strategies have to be employed for adaptation to these changes. This study, exemplifying coffee, showed that agroforestry has the required potential first to strongly buffer heat-shocking canopy temperature maxima by 2.5°C, *i.e.* a significant part of predicted temperature increments. Management, yield and economy of this process were already known and experienced for decades, ensuring a secure and reactive implementation with low required investments for small-holders. The quantitative study and models proposed here support and should ease future decisions on cropping designs adapted to climate changes. Agroforestry appears to be an effective and non-reclusive adaptation option, remaining fully compatible with longer-term strategies, such as breeding and grafting, and providing several other advantages for resilience than just microclimate.

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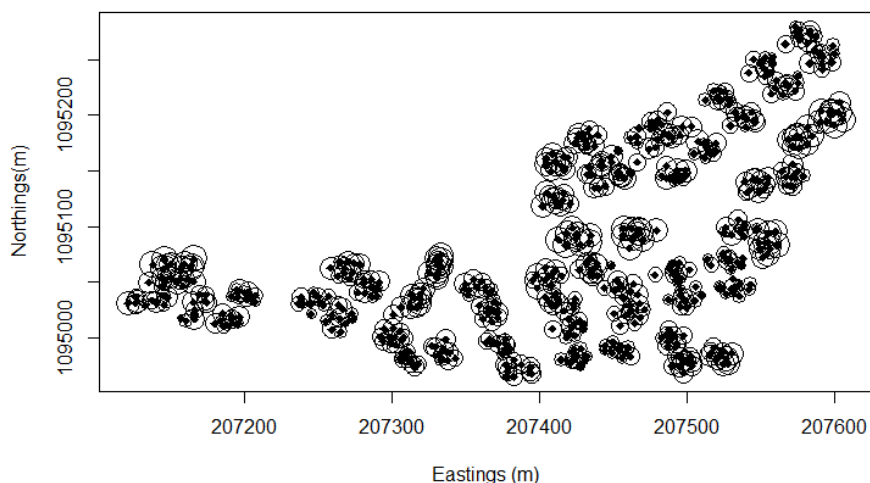
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### Suppl. Material I:

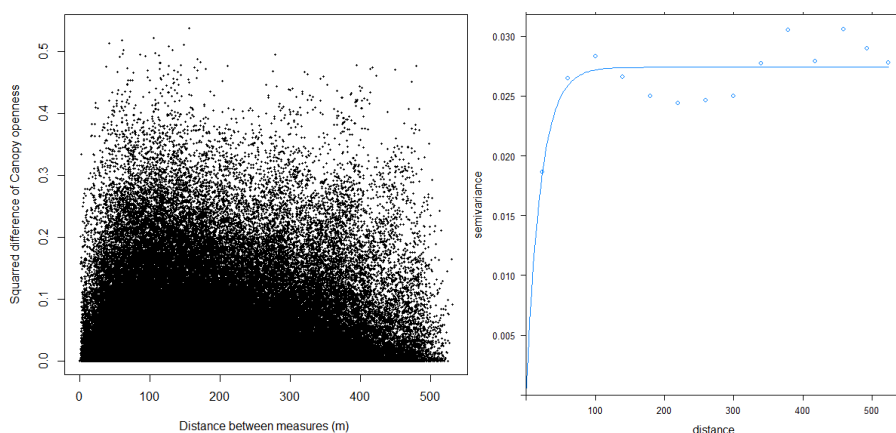
Groups of "Shade" x "Management" available for applying the method of contrasts, in order to guarantee statistical balance. Groups balanced for ●: MC, ■: IC+MC, ◆: IC+MC+IO, ★: MC+IO, ▲: IC+MC+IO+LO. Only MC was in common to every Shade and FS treatments.

Shade	Management			
C ●★	-	MC	IO	-
C+E ●■◆★▲	IC	MC	IO	LO
C+T ●★	-	MC	IO	-
T+E ●★	-	MC	IO	-
T ●■◆★	IC	MC	IO	-
E ●■◆★▲	IC	MC	IO	LO
FS ●■	IC	MC	-	-

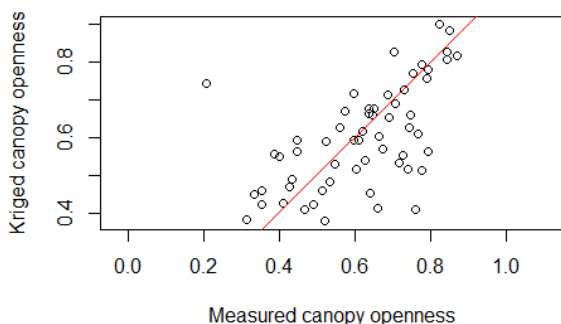
**Supplementary Material II**



a: Distribution of canopy openness measurements (see APPENDIX I for corresponding position of treatments). Circles are proportionnal to canopy openness values. N=570 measurements. It is observable that circles are systematically distributed over the trial.



b: (left) variographic cloud of canopy openness. During the first 40m of distance between points, the difference of canopy openness increased. Kriging condition is validated; (right): semi-variogram of exponential type (blue line) modelled for canopy openness variance. Points are measured values.



c: Cross-validation of 57 measured canopy openness (10% of dataset). Red line is the identity function







# Annexe 2

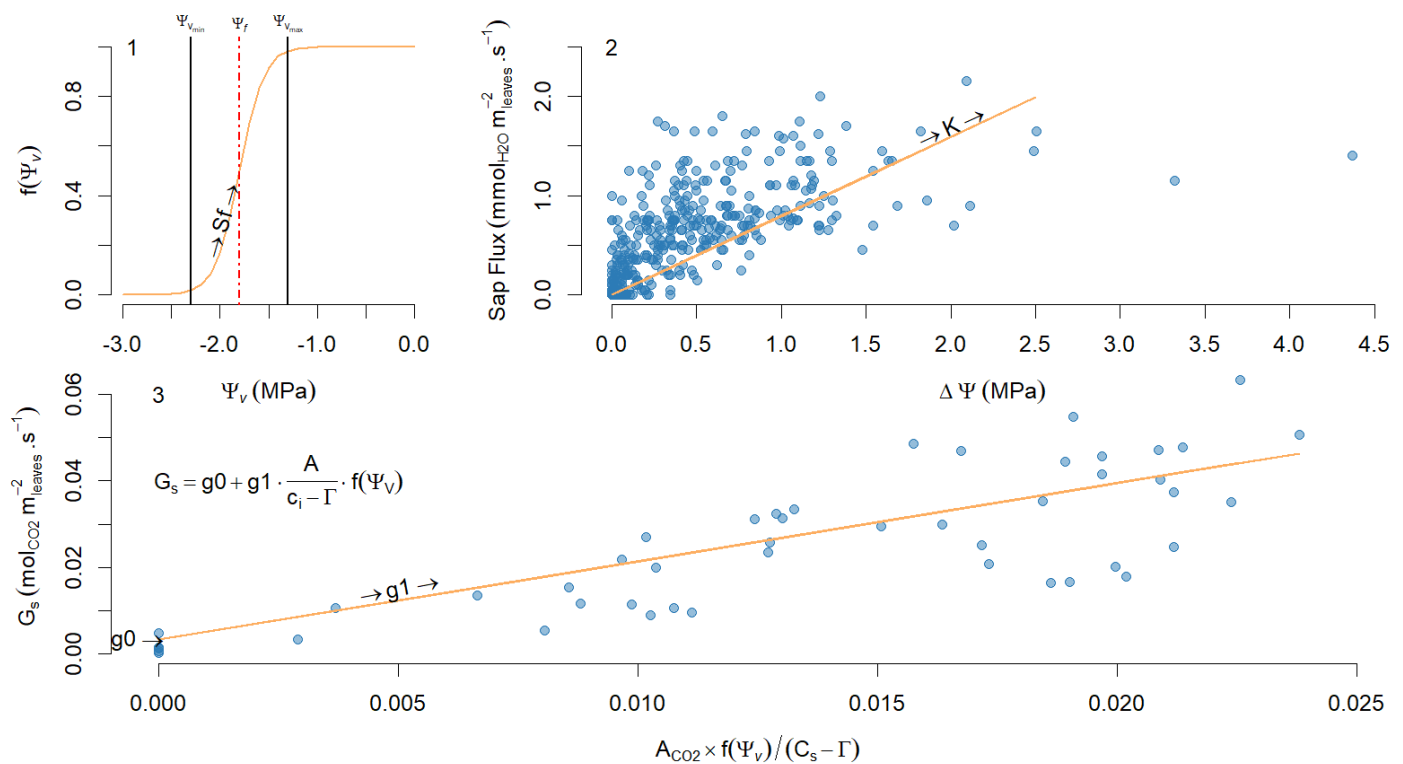


Figure A1. Tuzet et al. (2003) conductance model parameterization using 6 *Coffea* sprouts sap fluxes and leaf water potential. (1)  $Sf$  and  $\Psi_f$  parameters fit using data  $\Psi_{min}$  and  $\Psi_{max}$  data from (Dauzat et al., 2001) ; (2) Root-to-leaf plant conductivity ( $K$ ) and (3)  $G_0$  and  $G_1$  parameters fitting.

**Table A1** *Eucalyptus* parameters for MAESPA model parameterization.

Names	and	Symbol	Value	Unit	Source
<b>Photosynthetic</b>					
Max. rate of electron transport	top canopy	$J_{MAX}$	172.1	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Christina et al. (2017)
	middle		141.5		
	bottom		92.9		
Max. rate of Rubisco activity	top canopy	$V_{CMAX}$	66.9	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Christina et al. (2017)
	middle		68.3		
	bottom		57.3		
Dark respiration parameter	top canopy	Rd	1.69	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Christina et al. (2017)
	middle		1.62		
	bottom		1.53		
Quantum yield		$\alpha$	0.38	$\text{mol mol}^{-1}$	
Curvature parameter		$\theta$	0.53	unitless	
<b>Canopy water balance</b>					
Maximum	canopy	S	0.21	mm	Maquere (2008)
<b>Parameters for Stomatal conductance</b>					
Min.stomatal conductance	low	$g_{01}$	0.021	$\text{mol m}^{-2} \text{s}^{-1}$	Battie-Laclau et al. (2014)
	high	$g_{02}$	-0.337	$\text{mol m}^{-2} \text{s}^{-1}$	
Conductance slope		$g_{11}$	4.681	unitless	
Conductance slope		$g_{12}$	21.657	unitless	
Sensitivity parameter		Sf	2.253	$\text{MPa}^{-1}$	
Bulk Plant	leaf water	$\Psi_f$	-2.899	MPa	Christina et al. (2015)
	water	Kp	1.21	$\text{mmol m}^{-2} \text{s}^{-1}$	
<b>Soil-canopy aerodynamic conductance</b>					
Wind measurement		$z_{ht}$	30	m	Christina et al. (2017)
Zero-plane		$z_{0ht}$	0.01	m	Choudhury and Monteith (1988)
Min. thickness of the		$\alpha_0$	0.001	m	
<b>Root parameters</b>					
Maximum rooting		$a_R$	16.61	m	Christina et al. (2011)
		$b_R$	0.00202	$\text{day}^{-1}$	
		$c_R$	1.5883	unitless	
Specific root length	18 months	SRL	26.7	$\text{m g}^{-1}$	Christina et al. (2015)
	42 months		19.8		
Root mass density	4 months	RMD	40	$\text{g m}^{-2}$	Christina et al. (2011) and Christina et al. (2017)
	10 months		202		
	18 months		321		
	30 months		717		
	42 months		789		

**Table A2** *Coffea* parameters for MAESPA model parameterization.

Names and definition	Symbol	Value	Unit	Source
<b><i>Photosynthetic parameters</i></b>				
Max. rate of photosynthetic electron	$J_{MAX}$	88.21	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Charbonnier et al. (2013)
Max. rate of Rubisco carboxylase	$V_{CMAX}$	44.06	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Charbonnier et al. (2013)
Dark respiration	Rd	0.1752	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Charbonnier et al. (2013)
Quantum yield of electron transport	$\alpha$	0.222	$\text{mol mol}^{-1}$	Charbonnier et al. (2013)
Curvature parameter	$\theta$	0.96	unitless	Charbonnier et al. (2013)
<b><i>Canopy water balance</i></b>				
Maximum canopy storage	S	0.2	mm	Empirical coefficient
<b><i>Stomatal conductance</i></b>				
Minimum stomatal conductance	$g_0$	0.0033	$\text{mol}_{\text{CO}_2} \text{m}^{-2} \text{s}^{-1}$	This study
Empirical coefficient	$g_1$	1.809	unitless	This study
Sensitivity parameter	Sf	8	$\text{MPa}^{-1}$	Dauzat et al. (2001)
Bulk leaf water potential	$\Psi_f$	-1.8	MPa	Dauzat et al. (2001)
Plant water conductivity	K	0.7946	$\text{mmol m}^{-2} \text{s}^{-1} \text{MPa}^{-1}$	This study
Minimum water potential	$\Psi_{\text{min}}$	-2.3	MPa	Dauzat et al. (2001)
<b><i>Soil aerodynamic conductance</i></b>				
Wind measurement height	$z_{\text{ht}}$	3	m	This study
Soil zero-place displacement	$z_{0\text{ht}}$	0.01	m	Choudhury and Monteith (1988)
Min. thickness of the soil surface dry		0.001	m	
<b><i>Root parameters</i></b>				
Specific root length	SRL	26.733	$\text{m g}^{-1}$	Defrenet et al. (2016)
Root mass density	RMD	3550.5	$\text{g m}^{-2}$	Defrenet et al. (2016)



## Annexe 3

### **Simulating the effects of contrasted potassium and water supply regimes on soil water content and water table depth over the development of tropical *Eucalyptus grandis* plantations**

Christina M.<sup>1,2</sup>, le Maire G.<sup>1,3</sup>, Nouvellon Y.<sup>1,4</sup>, Vezy R.<sup>1,5</sup>, Bordon B.<sup>6</sup>, Battie-Laclau P.<sup>1,7</sup>, Gonçalves, J.L.M.<sup>6</sup>, Delgado-Rojas, J.S.<sup>6</sup>, Bouillet J-P<sup>1,6</sup>, Laclau J.-P.<sup>1,6,8</sup>

<sup>1</sup> CIRAD, UMR Eco&Sols, F-34398 Montpellier, France

<sup>2</sup> CIRAD, UR 115 AIDA, 2 Avenue Agropolis, 34398 Montpellier, France

<sup>3</sup> NIPE, UNICAMP, Campinas, Brazil

<sup>4</sup> Universidade de São Paulo, Departamento de Ciencias Atmosfericas, SP, Brazil

<sup>5</sup> INRA, UMR 1391 ISPA, F-33140 Villenave d'Ornon, France

<sup>6</sup> Universidade de São Paulo, ESALQ, Piracicaba, SP, Brazil

<sup>7</sup> Universidade de São Paulo, CENA, Piracicaba, SP, Brazil

<sup>8</sup> Universidade Estadual Paulista 'Júlio de Mesquita Filho', Departamento de Solos e Recursos Ambientais, CEP 18610-300 Botucatu, São Paulo, Brazil

Corresponding author: mathias.christina@cirad.fr

Present address: UPR AIDA, CIRAD, 2 Avenue Agropolis 34398 Montpellier Cedex 5, France

#### **Highlights**

- High fertilization rates increase trees water stress during drought
- A decrease in fertilization reduces tree water uptake in very deep soil layers
- Water recharge in deep soil layers is essential to reduce tree water stress
- Fertilization regimes can be a flexible tool to modify local trade-offs between wood production and soil water resources.

## Summary

Climate change is expected to increase the length of drought periods in many tropical regions. Although large amounts of potassium (K) are applied in tropical crops and planted forests, little is known about the interaction between K nutrition and water supply regimes (W) on water resources in tropical regions. Soil water availability in deep soil layers is likely to have a major influence on tree growth during dry periods in tropical planted forests. A process-based model (MAESPA) was parameterized in a throughfall exclusion experiment in Brazil to gain insight into the combined effects of K deficiency and rainfall reduction (37% throughfall exclusion) on tree water use, soil water storage and water table fluctuations over the first 4.5 years after planting *Eucalyptus grandis* trees. A comparison of canopy transpiration in each plot with the values predicted if the same soil was maintained at field capacity made it possible to compute a soil-driven tree water stress index in each treatment. Relative to K-fertilized trees under undisturbed rainfall (+K+W), canopy transpiration was 40% lower under K-deficiency (-K+W), 20% lower under W deficit (+K-W) and 36% lower under combined K deficiency and W deficit (-K-W) on average. Water was withdrawn in deeper soil layers in -W than in +W, particularly over dry seasons, while water withdrawal was more superficial in -K than in +K. Mean soil water contents down to a depth of 18 m were 24% higher in -K+W than in +K+W from 2 years after planting onwards (after canopy closure), while they were 24% and 12% lower in +K-W and -K-W, respectively, compared to +K+W. The soil-driven tree water stress index was 166% higher over the first 4.5 years after planting in -W relative to +W, 76% lower in -K relative to +K, and 14 % lower under -K-W relative to +K+W. Over the study period, deep seepage was higher by 371 mm yr<sup>-1</sup> (+122%) in -K relative to +K plots and lower by 200 mm yr<sup>-1</sup> (-66%) in -W relative to +W plots. Deep seepage decreased by 44% under combined -K and -W in comparison with +K+W. At the end of the study period, our modeling approach predicted a shallower level of the water table under K deficient trees (depth of 10 m in -K+W and 16 m in -K-W) than under K-fertilized trees (16 m in +K+W and 18 m in +K-W). Our study suggests that flexible fertilization regimes could contribute to adjusting the local trade-off between wood productions and soil water resources in planted forests.

**Keywords:** water resources; water table; groundwater; Brazil; *Eucalyptus*; deep roots; nutrients



## 1. Introduction

Planted forests provided 46% of the wood consumption worldwide in 2012, and 65% in tropical and subtropical regions (Payn et al., 2015). Their contribution to satisfying the global wood demand should increase in the future (Paquette and Messier, 2010). However, climate change is expected to exacerbate the intensity and frequency of future droughts in tropical and subtropical regions (Allison et al., 2009; IPCC, 2013; Solomon et al., 2009). Fast-growing tropical plantations require large amounts of water and are, consequently, particularly vulnerable to changes in rainfall patterns (Allen, 2009). The sustainability of fast-growing planted forests in a context of extended dry periods in many tropical regions will probably require a revision of management strategies to improve tree tolerance to drought (Battie-Laclau et al., 2014a, 2016; Carter and White, 2009).

Water storage in deep soil layers is likely to strongly influence tree functioning in tropical regions (Malhi et al., 2008). Indeed, water uptake by deep roots is generally considered as an efficient adaptation to drought in tropical forests that maintains transpiration rates during dry periods by withdrawing water from soil depths > 8–10 m (Christina et al., 2017; Markewitz et al., 2010; Nepstad et al., 1994). Water uptake at the capillary fringe above the water table is likely to account for a substantial proportion of tree water use in eucalypt forests (Dawson and Pate, 1996; Zolfaghar et al., 2014; Eamus et al., 2015), even under relatively high rainfall regimes (approx. 1500 mm yr<sup>-1</sup>) for water tables at depths between 10 m and 18 m (Christina et al., 2017). Recent studies showed that tree water stress and mortality in Australian eucalypt forests are dependent on the amount of water stored in deep soil layers (Harper et al., 2009; Brouwers et al., 2013; Zolfaghar et al., 2014). The same behavior was observed in Amazonian Forest (da Costa et al., 2010; Malhi et al., 2009) and in Brazilian savanna (Jackson et al., 1999; Oliveira et al., 2005). In consequence, modifications of the current management practices in drought-prone planted forests have been proposed to decrease tree water stress during dry periods. The most common silvicultural adaptations proposed are: i) to plant species and hybrids selected by breeding programs for their high tolerance to drought (Dutkowski et al., 2012; Rojas et al., 2017), ii) to decrease the stocking densities (Mendham et al., 2011; White et al., 2009) or rotation lengths (Harper et al., 2014), iii) to reduce the amounts of fertilizer applied (Forrester et al., 2013; Battie-Laclau et al., 2014a; White et al., 2009), and iv) to concentrate the future afforestation programs on deep soils (Harper et al., 2014; Battie-Laclau et al., 2016).

Although the positive effects of an adequate nutritional status on plant resistance to abiotic stresses (Cakmak, 2005; Reddy et al., 2004), carbon partitioning to wood production (Litton et al., 2007; Epron et al., 2012), and water-use efficiency (White et al., 2014; Battie-Laclau et al., 2016) are well established, some studies also showed that fertilization is likely to increase tree water stress during dry periods (Linder et al., 1987; White et al., 2009). Measurements (Battie-Laclau et al., 2014a, 2016) as well as modeling approaches (Christina et al., 2015) in a field experiment manipulating throughfall and potassium (K) supply showed that a decrease in K fertilizer relative to current doses in commercial eucalypt plantations might help reduce tree water stress during drought through lower water-use and increased water storage in deep soil layers during rainy seasons.

Concerns have been raised over the last decades about the impact of a highly productive eucalypt plantations on groundwater resources and stream flow in tropical regions (Cossalter and Pye-Smith, 2003; Farley et al., 2005). In a future drier climate, management practices should be adapted to maintain wood production while limiting adverse consequences on groundwater resources. Our study aimed to gain insight into the effects of contrasting K and water supply regimes on tree water use and water seepage under highly productive *Eucalyptus* plantations in tropical soils. We hypothesized that: i) a decrease in rainfall reduces tree water use and the recharge of the water table, but increases tree water stress and the depth of water uptake in the soil and ii) a decrease in fertilization could mitigate the adverse consequences of low precipitation regimes on tree water stress and soil water resources.

## 2. Material & Methods

### 2.1. Site description

The experiment was conducted at the Itatinga Experimental Station of the University of São Paulo in Brazil (23° 020S; 48° 380W). From 2010 to 2014, the mean annual precipitation was 1578 mm yr<sup>-1</sup>, with a drier year in 2014 (1189 mm yr<sup>-1</sup>) at this site. The dry season lasted from June to September with a mean monthly temperature of 15 °C, and the rainy season was from October to May, with a mean monthly temperature of 25 °C and higher overall PAR. The experiment was located on a hilltop (slope <3%) at an altitude of 850 m. The soils were very deep Ferralsols (>15 m; Christina et al., 2011) developed on Cretaceous sandstone, with clay content ranging from 14% in the top soil to 23% in deep soil layers and mean concentrations of exchangeable K ranging from 0.02 cmolc kg<sup>-1</sup> in the upper soil layer and <0.01 cmolc kg<sup>-1</sup> between the depths of 0.05 m and 15 m (Laclau et al., 2010).

The experiment was described in detail by Battie-Laclau et al. (2014a). A split-plot experimental design was set up in June 2010 with a highly productive *E. grandis* clone used in commercial plantations by the Suzano Company (São Paulo, Brazil). Two fertilization regimes (+/-K) and two water supply regimes (+/-W) were applied in three blocks. The area of individual plots was 864 m<sup>2</sup> (144 trees per plot). The four treatments were:

- +K+W: a fertilization with K (0.45 mol K m<sup>-2</sup> applied as KCl) and no throughfall exclusion,
- -K+W: no K addition and no throughfall exclusion,
- +K-W: K addition and c. 37% of throughfall exclusion,
- -K-W: no K addition and c. 37% of throughfall exclusion.

Potassium fertilizer was applied 3 months after planting and did not limit tree growth at our study site (Almeida et al., 2010). Other nutrients were applied at planting for all treatments (3.3 g P m<sup>-2</sup>, 200 g m<sup>-2</sup> of dolomitic lime and trace elements) and at 3 months after planting (12 g N m<sup>-2</sup>), which was non-limiting for tree growth at this study site (Laclau et al., 2009). Throughfall was excluded using panels made of clear, PAR-transmitting greenhouse plastic sheets mounted on wooden frames at a height of 1.6–0.5 m.

Meteorological data were obtained from June 2010 to December 2014 using an automatic station placed at the top of a 21-m high tower located at 50 m from the experiment. The following data were used as inputs to the MAESPA model: incident total short-wave radiation (RAD,  $\text{W m}^{-2}$ ), air temperature ( $T_{\text{air}}$ ,  $^{\circ}\text{C}$ ), relative humidity (RH, %), atmospheric pressure (Press, Pa), wind speed above the canopy (Wind,  $\text{m s}^{-1}$ ) and precipitation (PPT, mm). Annual precipitations were 1834, 1622, 1714 and 1103  $\text{mm yr}^{-1}$  in 2011, 2012, 2013 and 2014 (exceptionally dry year), respectively.

Measured canopy transpiration was estimated using sap flow measurements (see Battie-Laclau et al., 2016 for details). The sap flow density was measured from July 2011 to June 2013 in 10–13 trees in each treatment at a 30-min time step, using a calibration equation determined in a preliminary study (Delgado-Rojas et al., 2010). In each treatment, a linear regression was performed between the daily sap flow of each tree and the circumference at breast height (CBH). These regressions were then used to estimate the daily stand-scale canopy transpiration from the CBH of all the trees in each inner plot. Soil water content was measured with 3 TDR probes (Trase Soilmoisture, Santa Barbara, CA, USA) at the depths of 0.5, 1.5, 3.0, 4.5 and 6.0 m over the study period.

## 2.2. MAESPA presentation

The MAESPA model (Duursma and Medlyn, 2012) is a model coupling the above-ground components of the MAESTRA model (Medlyn et al., 2007; Wang and Jarvis, 1990) and the water balance components of the SPA model (Williams et al., 2001a,b), with several changes and additions (Christina et al., 2017). The model has a long history of development and applications on diverse forest types (see the bibliography at <http://maespa.github.io/bibliography.html>). A 3D single-tree based model calculates light interception and distribution within the tree crowns to estimate the absorbed photosynthetically active radiation for individual trees in the stand, considering neighboring trees that compete for light. A leaf physiology model is used to estimate photosynthesis and transpiration at the leaf scale (Medlyn, 1998). The water balance is based on a soil-root-leaf-air water potential gradient and on the hydraulic conductivity between these compartments. Transpiration is calculated from the Penman-Monteith equation applied to small volumes of leaves. The leaf water potential, which is used to calculate the leaf stomatal conductance (Tuzet et al., 2003), is adjusted to ensure that the Penman-Monteith estimation of transpiration matches the total water flow computed from the soil-plant-air water potential gradient. The soil is considered as horizontally uniform. Water uptake is distributed between the soil layers depending on the fine root density and soil water potential. The soil water storage in each layer is calculated as the budget between infiltration, soil evaporation, drainage, root water uptake, capillary rising and lateral flow from the water table. The fraction of roots in each layer is an input parameter in the model as well as root characteristics such as root diameter, specific root length and total root biomass. Root systems are assumed to be homogeneous under the whole stand. Details of equations and mechanisms driving the water balance were described in Duursma and Medlyn (2012) with some modifications detailed in Christina et al. (2017; supplementary information).

### 2.3. MAESPA parameterization

The MAESPA model has been parameterized over the first 3 years after planting for the studied site (split-plot design crossing K and water supply regimes, Christina et al., 2015, appendix Table A2). In addition, leaf area index, crown morphology, tree height and leaf angle measurements were extended in all the treatments until 4.5 years after planting using the methods described in Christina et al. (2015). Belowground model parameters are given in appendix (Table A3). We assumed that soil hydraulic conductivity decreased linearly with depth between 3 and 8 m, and remained constant below this threshold. In each treatment, the minimum soil water content for root absorption was the lowest volumetric water content measured by TDR probes at each depth over the study period (Christina et al., 2015) and we assumed a linear increase with soil depth down to 18m depth (as in Christina et al., 2017). The soil profile is divided in 50-cm thick soil layers down to 18 m depth, with specific soil characteristics and root densities in each layer.

The experiment was established close to a hilltop and monthly measurements of the water table level showed that it fluctuated throughout the first 4.5 years after planting between the depths of 15 m and 17 m, with small differences between treatments. Large amounts of deep drainage in a neighbor stand of very low leaf area index (LAI) at the top of the hill influenced the level of the water table within the experiment, with a rise of 1–2 m at the end of each rainy season independently of the treatment. The small area of each treatment within the field trial did not make it possible to measure the effects of the K and W supply regimes on the water table depth in each treatment. For this, very large stand would have been necessary, which was not technically possible. A modeling approach was therefore used to explore the impact of these treatments on the water table present in each plot at the same depth at planting, and to assess the consequences of K nutrition and contrasted water supply regimes on soil water resources in *Eucalyptus* plantations, as it would happen in commercial plantations covering large areas. We used in our simulations the initial depth and the groundwater lateral flow parameter of the water table measured in a large nearby commercial *Eucalyptus* plantation. It is a 90 ha stand growing on the same soil type and studied in detail in Christina et al. (2017). All the other parameters used in the MAESPA model (soil and plant parameters) were specifically determined from measurements in the experiment manipulating K and W supply regimes, as described above (appendix Table A1, A2 & A4). Measurements in the large commercial stand showed that the water table was at an initial depth of 18.5 m at planting and had a lateral flow of  $\sim 0.5 \text{ mm d}^{-1}$  (Christina et al., 2017). Finally, simulations were performed for the 36 inner trees in each plot over 4.5 years after planting and at a 15-min time step with the MAESPA model. Six lines of trees were added as buffer rows in the simulations to take into account the radiation environment of the 36 target trees.

### 2.4. MAESPA simulations and comparison with measurements

Daily transpiration was estimated for each tree and cumulated for the whole inner plots of each treatment. It was then divided by the area of the inner plots to estimate a stand-scale canopy transpiration ( $T_C$ ,  $\text{mm d}^{-1}$ ). The

depths of water uptake were weighted daily by the fraction of transpiration withdrawn in each soil layer to estimate the weighted uptake depth ( $D_{UPT}$ , m). For one particular day, the weighted uptake depth was calculated as follows:

$$D_{UPT} = \frac{\sum_i D_i * UPT_i}{\sum_i UPT_i}, \quad (1)$$

where  $UPT_i$  is the amount of water withdrawn in layer  $i$  ( $\text{mm d}^{-1}$ ), and  $D_i$  is the depth of layer  $i$  (m) from the soil surface to the depth of the water table (defined as the upper depth where the soil water content was at saturation). Water uptake in the capillary fringe of the water table was considered.

A soil-driven water stress index was computed to assess the consequences of soil water limitation on tree water status. We simulated the stand-scale canopy transpiration over the 4.5 years of growth with a soil water content forced at saturation throughout the soil profile ( $T_{C,sat\_soil}$ ), while all other parameters were identical to the simulation with non-forced soil water contents.  $T_{C,sat\_soil}$  was influenced by canopy structural characteristics (e.g. leaf area index, leaf angles, tree position and sizes), by meteorological conditions (e.g. global radiation, vapor pressure deficit) but not by soil water conditions. As a consequence,  $T_C$  is always lower (i.e. soil-driven water stress) or equal to  $T_{C,sat\_soil}$  (i.e. no soil-driven water stress). A daily soil-driven water stress index ( $I_{SWS,d}$ ) was therefore implemented based on the ratio between daily  $T_C$  and daily  $T_{C,sat\_soil}$  :

$$I_{SWS,d} = 1 - \frac{T_C}{T_{C,sat\_soil}}, \quad (2)$$

Similarly, a total soil-driven water stress index over the whole growth was computed as follows:

$$I_{SWS,tot} = 1 - \frac{\sum_i T_{C,i}}{\sum_i T_{C,sat\_soil,i}}, \quad (3)$$

Where,  $T_{C,i}$  and  $T_{C,sat\_soil,i}$  are the  $T_C$  and  $T_{C,sat\_soil}$  at day  $i$  (from planting date to 4.5 years), respectively.

Total deep seepage was computed as the sum of the groundwater lateral flow over the first 4.5 years after planting and the amount of water stored in the water table at age 4.5 years (difference between final and initial water content in saturated soil layers above a depth of 18.5). The deep seepage corresponds to the part of the water that will be for a large part available for stream flow at a time (blue water). Canopy transpiration, soil water content, weighted water uptake depth, deep seepage and water storage throughout the soil profiles were simulated for each plot of the split-plot experiment and averaged per treatment.

The model outputs for canopy transpiration ( $T_C$ ) and soil water content ( $\theta$ ) were compared to measurements made at the same site. Daily  $T_C$  simulations in each treatment were compared to sap flow measurements carried out by Battie-Laclau et al. (2016) from 1 to 3 years after planting.

### 3. Results

#### 3.1. Comparison between predicted and measured stand transpiration and soil water content

Predicted canopy transpiration time series fitted generally well the measurements (Fig. 1). Root mean square errors (RMSE) between daily measurements and simulations ranged from 0.63 to 1.08  $\text{mm d}^{-1}$ , depending on treatment. Over the two years of measurements, canopy transpiration was underestimated by 6 and 16% in +K+W and +K-W respectively, and was over-estimated by 9 and 15% in -K+W and -K-W.

There was an overall good agreement between simulated and measured soil water contents ( $\theta$ ) over the study period, whatever the treatment and the soil depth (Fig 2). The RMSE between simulated and measured  $\theta$  over the first 4.5 years after planting, across all the soil depths equipped with TDR probes, were similar in all treatments (RMSE = 0.020 - 0.023  $\text{m}^3 \text{m}^{-3}$ ). Small discrepancies between measured and simulated  $T_C$  and  $\theta$  (down to a depth of 6 m) in all the treatments suggest that our simulations of water fluxes throughout the soil profiles were realistic.

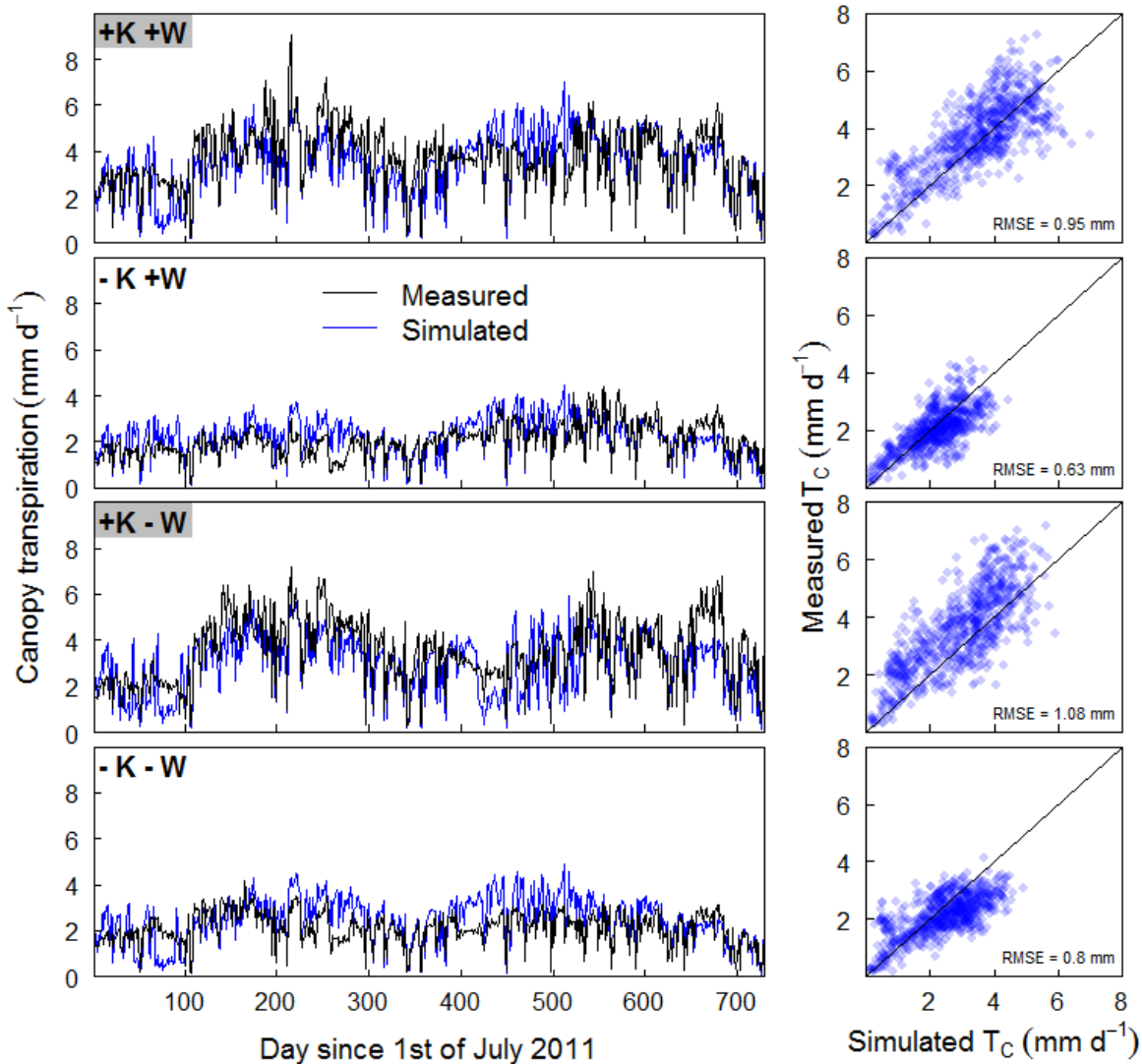


Fig. 1. Comparison between daily simulated (blue line) and measured (black line) canopy transpiration from 1 to 2 years after planting in *Eucalyptus grandis* plantations under four contrasting potassium (K) and water (W) availabilities. -K and +K refer to the K-deficient and K-supplied trees, respectively. +W and -W refer to undisturbed rainfall and exclusion of 37% of throughfall, respectively.

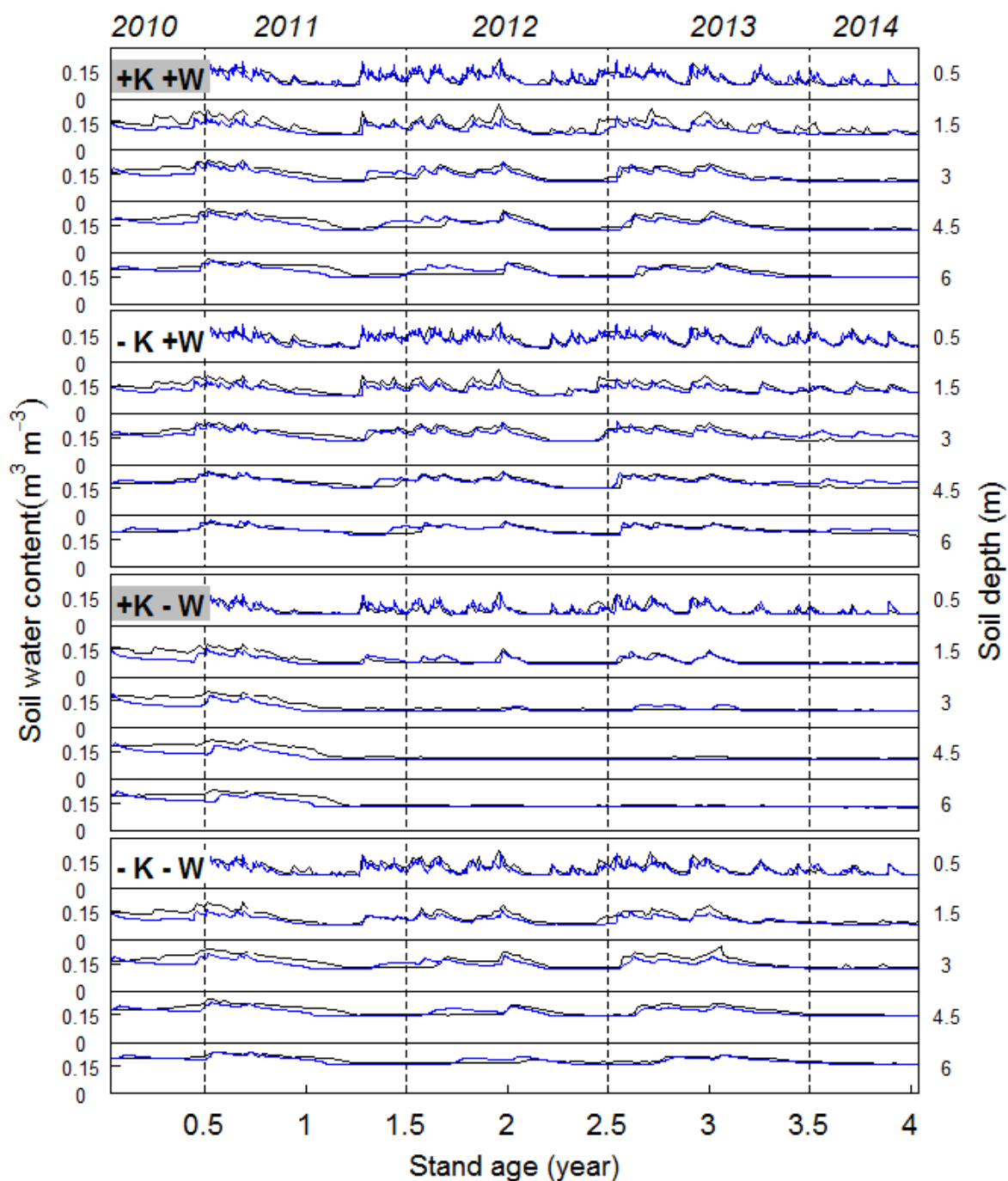


Fig. 2. Time course of simulated (blue line) and measured (black line) daily volumetric soil water content ( $\theta$ ) over the first 4 years after planting *Eucalyptus grandis* trees under contrasting potassium (K) and water (W) supply regimes.  $\theta$  was measured in each treatment at different depths (0.5m, 1.5m, 3m, 4.5m and 6m) using TDR probes. -K and +K refer to the K-deficient and K-supplied trees, respectively. +W and -W refer to undisturbed rainfall and exclusion of 37% of throughfall, respectively.

### 3.2. Canopy transpiration and tree water stress

The effects of K and W supply regimes on canopy transpiration ( $T_C$ ) changed over tree growth (Fig. 3). In +K+W,  $T_C$  sharply increased after planting up to approximately  $3 \text{ mm d}^{-1}$  at one year of age, then reached maximum values of  $5\text{--}6 \text{ mm d}^{-1}$  in the successive rainy seasons.  $T_C$  in +K+W was about half in dry season relative to rainy season. While time series of simulated  $T_C$  in +K-W were similar to those in +K+W the first year after planting,  $T_C$  was thereafter limited to maximum values of about  $4 \text{ mm d}^{-1}$  in +K-W over the rainy seasons. Under K deficiency (in -K+W and -K-W),  $T_C$  increased up to  $2 \text{ mm d}^{-1}$  the first year after planting and remained lower than  $3 \text{ mm d}^{-1}$  over the first 4.5 years. The effects of K deficiency and W deficit on  $T_C$  were therefore more pronounced after canopy closure (at about 1.5 years of age) than earlier. Throughfall exclusion led to a decrease in  $T_C$  ranging from 270 to  $517 \text{ mm y}^{-1}$  over growth in +K-W relative to +K+W after canopy closure (Table 1), which represented a global decrease by 20% over the first 4.5 years after planting (Fig. 5a). K deficiency in -K+W and both K deficiency and water deficit in -K-W led to similar values of daily  $T_C$ , with a decrease in both cases ranging from 231 to  $685 \text{ mm y}^{-1}$  over growth relative to +K+W (Table 1), which represented a global decrease by 38% (Fig 5a).

Only short periods with daily soil-driven tree water stress ( $I_{\text{SWS,d}}$ ) values  $> 0.2$  were simulated in +K+W over the study period, at the end of dry seasons (Fig 3). By contrast,  $I_{\text{SWS,d}}$  values were low in -K+W throughout tree growth, except during one short climatic event at about 1 year after planting.  $I_{\text{SWS,d}}$  values were high in each dry season in the +K-W treatment, and remained  $>0.4$  the majority of the days from 3.5 years onwards.  $I_{\text{SWS,d}}$  values in -K-W were slightly lower than in +K+W over the study period, even the 4<sup>th</sup> year after planting which was particularly dry. *Eucalyptus* transpiration was reduced by more than 10% only when available soil water content on rooted layers was under  $0.02 \text{ m}^3 \text{ m}^{-3}$ , except for +K-W treatment, with a higher threshold value of  $0.04 \text{ m}^3 \text{ m}^{-3}$ .



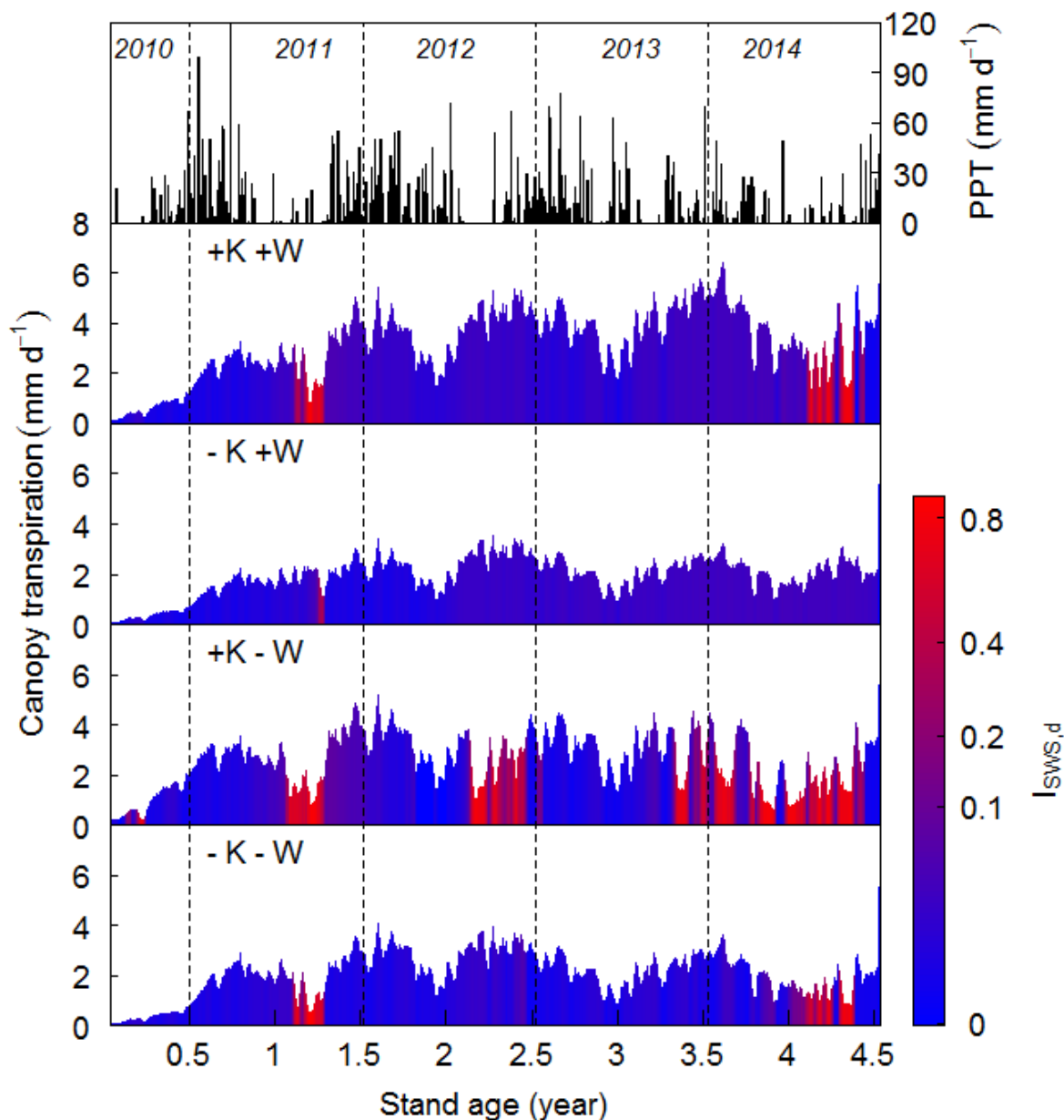


Fig. 3. Time-course of canopy transpiration ( $T_c$ ) in *Eucalyptus grandis* plots over 4.5 years after planting. -K and +K refer to the control and K-supplied trees, respectively. +W and -W refer to undisturbed rainfall and exclusion of 37% of throughfall, respectively. Corresponding relation between canopy transpiration and canopy transpiration with a non-limiting water content (daily soil-driven water stress index,  $I_{SWS,d}$ ) throughout the soil profile explored by tree roots is shown with a gradient of colour (red for transpiration limited by soil water storage, and blue for non-limited transpiration). Daily precipitation (PPT) over the study period is shown in the upper graph.

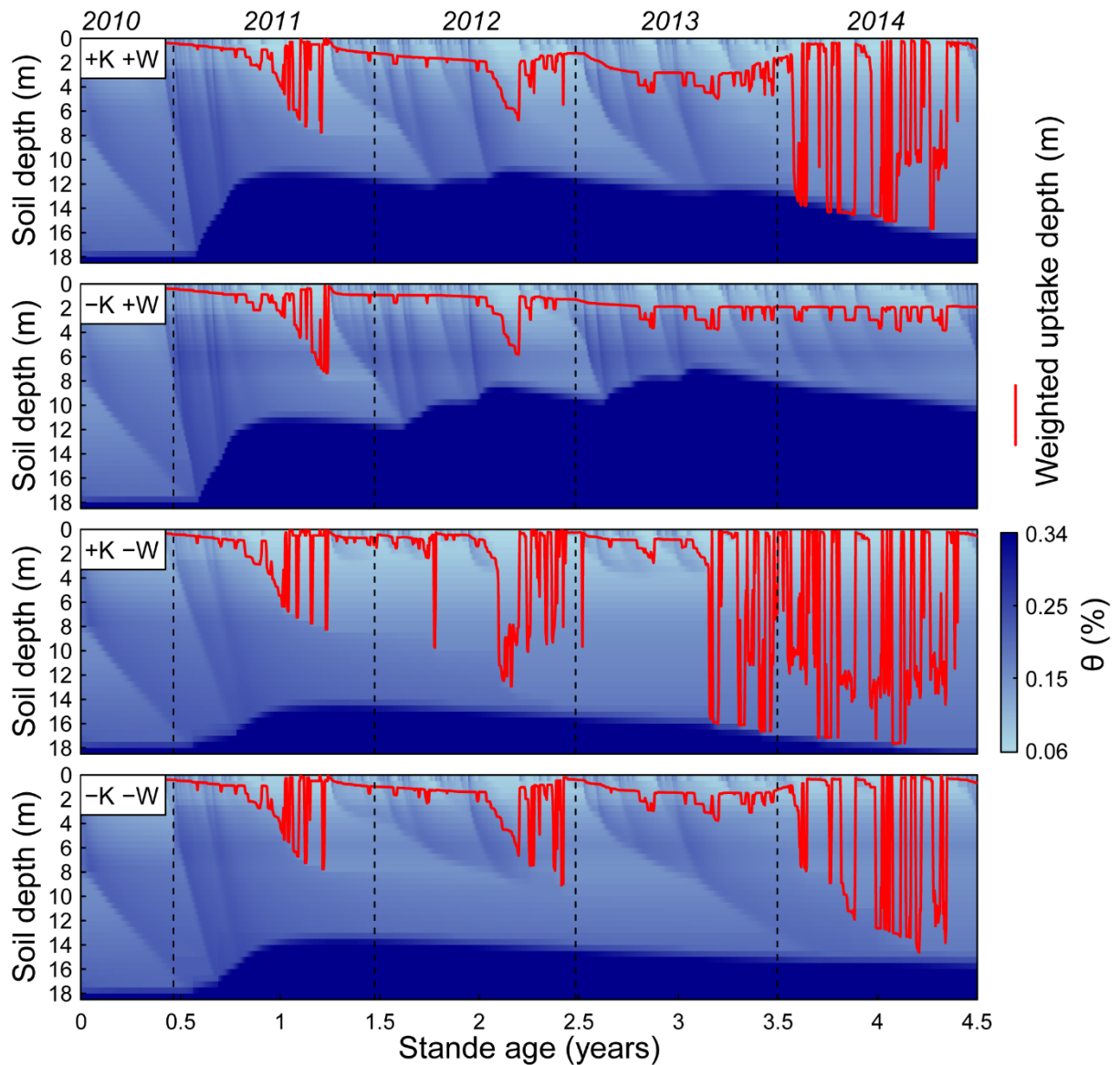


Fig 4. Daily simulated soil water content ( $\theta$ ,  $\text{m}^3 \text{m}^{-3}$ ) per soil layer down to a depth 18 m over 4.5 years after planting under undisturbed rainfall and K fertilization (+K+W) or in response to potassium deficiency (-K+W), water deficit (+K-W) and combined potassium deficiency and water deficit (-K-W). The red line indicates the daily weighted uptake depth (m).

The soil-driven tree water stress index ( $I_{\text{SWS,tot}}$ ) over the growth period (4.5 years) was strongly influenced by K and W supply regimes (Fig. 5b). In comparison with common fertilization practices (+K+W),  $I_{\text{SWS,tot}}$  was increased by 166% under throughfall exclusion for K-fertilized trees (in +K-W) and decreased by 76% under K deficiency (in -K+W). The combined effect of -K and -W showed a slightly lower  $I_{\text{SWS,tot}}$  (-14%) than in the reference treatment (+K+W). Lower  $I_{\text{SWS,tot}}$  values for K-deficient trees than K-fertilized trees was also observed in throughfall exclusion plots (in -K-W relative to +K-W).

**Table 1. Water fluxes over stand growth under contrasting potassium (+K vs -K) and rainfall (+W vs -W) supply regimes in *Eucalyptus grandis* plantations. Annual canopy transpiration and water uptake by trees at different depths (0-5m, 5m down to the water table, and at the capillary fringe of the water table) are distinguished for the first 4 years of growth. Annual values of soil water storage in vadose zone and groundwater lateral flows are shown. Annual precipitations were 1834, 1622, 1714 and 1103 mm yr<sup>-1</sup> from 0.5 to 1.5, 1.5 to 2.5, 2.5 to 3.5 and 3.5 to 4.5 year after planting, respectively.**

Stand age (year)	Canopy transpiration (mm yr <sup>-1</sup> )			
	+K+W	-K+W	+K-W	-K-W
0.5-1.5	947	654	984	716
1.5-2.5	1365	881	1095	1035
2.5-3.5	1438	753	1110	792
3.5-4.5	1323	774	806	705
<b>Uptake 0 – 5 m (mm yr<sup>-1</sup>)</b>				
	+K+W	-K+W	+K-W	-K-W
0.5-1.5	840	598	859	639
1.5-2.5	1115	798	955	872
2.5-3.5	1088	644	933	722
3.5-4.5	796	647	543	523
<b>Uptake 5 m – water table (mm yr<sup>-1</sup>)</b>				
	+K+W	-K+W	+K-W	-K-W
0.5-1.5	107	56	125	77
1.5-2.5	233	78	140	163
2.5-3.5	341	84	50	70
3.5-4.5	221	118	79	182
<b>Uptake in the water table capillary fringe (mm yr<sup>-1</sup>)</b>				
	+K+W	-K+W	+K-W	-K-W
0.5-1.5	0	0	0	0
1.5-2.5	17	5	0	0
2.5-3.5	9	25	127	0
3.5-4.5	306	9	184	0
<b>Vadose soil water storage (mm yr<sup>-1</sup>)</b>				
	+K+W	-K+W	+K-W	-K-W
0.5-1.5	+387	+614	-111	+106
1.5-2.5	-143	+241	-241	-248
2.5-3.5	-256	+220	-285	+2
3.5-4.5	-524	-208	-92	-157
<b>Groundwater lateral flow (mm yr<sup>-1</sup>)</b>				
	+K+W	-K+W	+K-W	-K-W
0.5-1.5	291	287	144	132
1.5-2.5	350	443	170	172
2.5-3.5	308	532	112	126
3.5-4.5	174	470	23	96

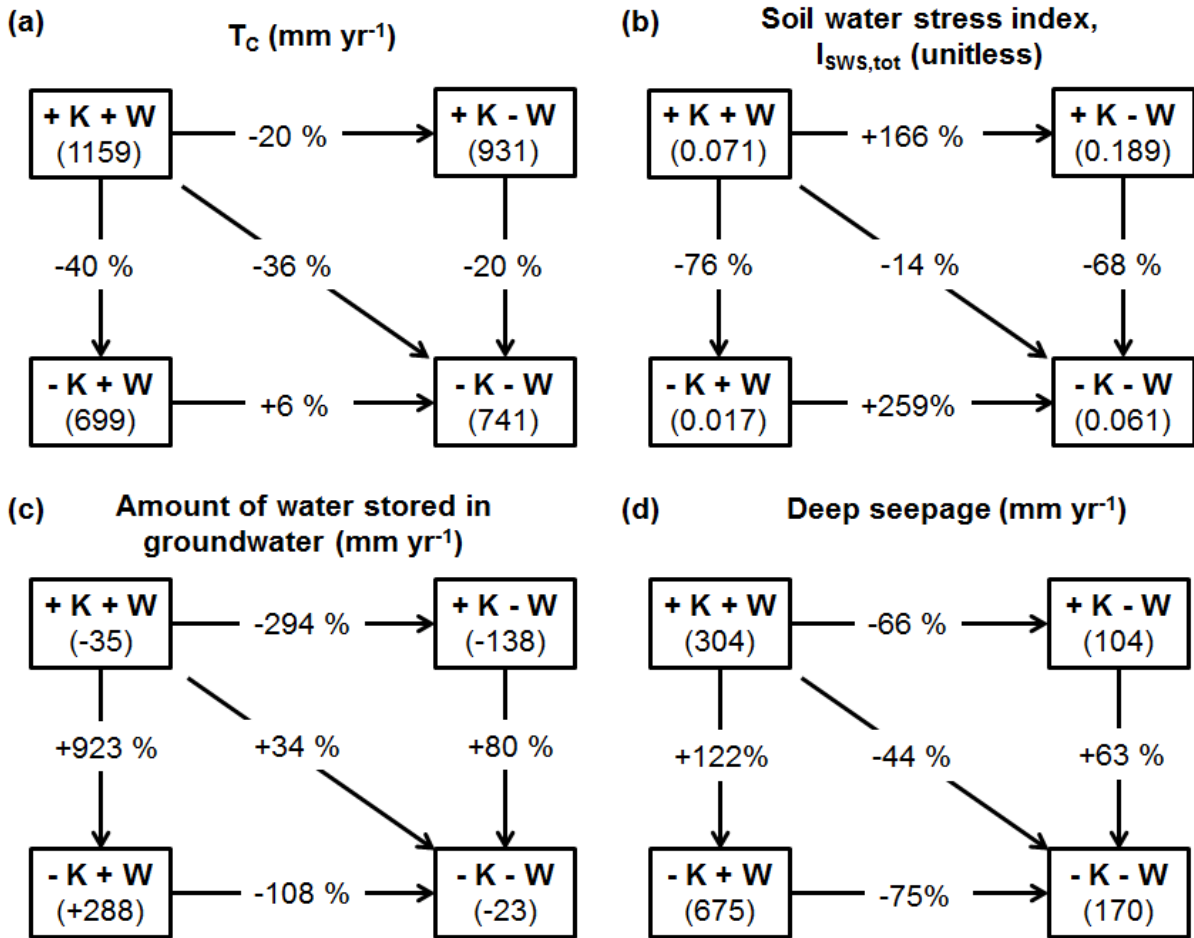


Fig. 5. Mean responses of eucalypt trees to contrasting potassium and water supply regimes over 4.5 years after planting: a) canopy transpiration ( $T_c$ , mm yr<sup>-1</sup>), b) soil water stress index ( $I_{SWS}$ , unitless), c) changes in amount of water stored in the groundwater down to a depth of 18m (mm yr<sup>-1</sup>) and d) deep seepage (sum of groundwater lateral flow and water stored in the water table, mm yr<sup>-1</sup>). The variations are shown in percentages on arrows and mean annual values are indicated within each box. -K and +K refer to the control and K-supplied trees, respectively. +W and -W refer to undisturbed rainfall and exclusion of 37% of throughfall, respectively.

### 3.3. Depth of water withdrawal

While contrasting K and W supply regimes strongly influenced annual  $T_c$ , the depth of water uptake was little affected by the treatments up to age 2 years (Fig. 4). However, water uptake depths sharply increased in K-fertilized stands the 4<sup>th</sup> year after planting, which was characterized by an exceptionally low rainfall at our study site (Table 1), with mean annual values of approx. 6 m in +K-W, 4 m in +K+W and about only 2 m in K-deficient stands (-K+W and -K-W). The variability in depth of water uptake was much lower all along the 4<sup>th</sup> year after planting in -K+W than in the K-fertilized treatments (+K+W and +K-W) and in -K-W. Water was withdrawn more deeply over dry seasons than rainy seasons, with little differences between treatments up to age 3 years (Fig. 4). Over the dry season of the 4<sup>th</sup> year after planting, the mean depth of water uptake was only about 2 m in -K+W (with a low temporal variability) whereas it reached 7–9 m in the other treatments (with a high temporal variability). Water withdrawal at the vicinity of the water table hardly ever occurred in

the K-deficient treatments even under throughfall exclusion (Fig. 4, Table 1). On the contrary, our simulations show that it occurred from 2.5 years onwards in the +K-W treatment and from 3.5 years onwards in the +K+W treatment, after drying the upper soil layers. However, one should keep in mind that the simulation of the water table depth was theoretical for a large stand and with determined a dynamic within the catchment similar to another site previously studied at 15 km apart. The implications of this modeling choice will be further discussed.

During the first 2.5 years of growth, 88% of the amount of water used by trees was taken up in the first 5 meters in all treatments (Table 1). During the 3<sup>rd</sup> year of growth, water uptake in the upper 5 m remained high in all treatments (84–91%) except for +K+W where 24% of water was taken up below 5 m. In comparison, the same year in the +K-W treatment, water uptake below 5 m represented only 16% of the total water use (but 11% at the water table vicinity). Simulations estimated the water uptake in the water table capillary fringe to reach 23% of tree water use the last year of growth (exceptionally dry year) in both -W treatments (+K-W and -K-W). On the contrary, even during an exceptionally dry year, water uptake in the water table was almost non-existent in -K treatments.

### 3.4. Soil water contents and storage of water in the water table

K and W supply regimes strongly influenced soil water content ( $\theta$ ) throughout the soil profiles explored by fine roots (Fig. 4).  $\theta$  values were simulated higher in -K+W than in +K+W and the differences increased with stand age. As expected, throughfall exclusion decreased  $\theta$  in +K-W and -K-W relative to +K+W. The depth of the groundwater over the first 4.5 years after planting was highly dependent on the fertilization and water supply regimes (Fig. 4 and 5c). While the amount of water stored in the groundwater down to a depth of 18 m decreased by 35 mm yr<sup>-1</sup> on average over the study period in the +K+W treatment, it decreased by 138 mm yr<sup>-1</sup> in +K-W and increased by 288 mm yr<sup>-1</sup> in -K+W. The amount of water stored in the groundwater down to a depth of 18 m only decreased by 23 mm yr<sup>-1</sup> under combined -K and -W.

Simulated water table depths were highly dependent on the K and W supply regimes (Fig. 4). The depth of the water table increased from 18 to 12 m the first year after planting in the two treatments under undisturbed rainfall (+K+W and -K+W). While the water table progressively decreased down to a depth of 16 m at 4.5 years after planting in +K+W, it increased up to a depth of 10 m in -K+W at the same age. In both treatments under throughfall exclusion (+K-W and -K-W), the water table rose up to a depth of about 14 m at age 1 year. The water table depth slowly decreased thereafter, down to a depth of 16 m in -K-W at age 4.5 years because of lateral flows of the water table, while it felt at a depth of 18 m in +K-W, as a result of additional water uptake in the capillary fringe just above the water table. Our simulations showed a recharge of the water table by gravitational waters during years with high rainfall amounts for K-fertilized trees, but not when during years with low rainfall (in +K-W and the 4<sup>th</sup> year after planting in +K+W). The amounts of water reaching the water table were much higher under K-deficient trees than under K-fertilized trees.

The deep seepage (Fig 5d) was computed as the sum of the lateral flow over the stand growth (Table 1) and the water stored in the water table at the end of the study period. It was a proxy of the soil water resources supplying on the long-term stream flow in afforested catchments. Compared to common silvicultural practices (+K+W), deep seepage increased by 371 mm yr<sup>-1</sup> (+122%) over the study period under K deficiency (-K+W) and it decreased by 200 mm yr<sup>-1</sup> (-66%) under throughfall exclusion (+K-W).

## 4. Discussion

### 4.1. Simulation reliability

The discrepancies between measured and predicted values were relatively small in our study for stand transpiration and soil water contents, which suggests that the effects of K and water supply regimes on soil water resources were reliably simulated. Nevertheless, canopy transpiration estimates might be affected by several sources of uncertainty such as a rough estimation of the time-course of Leaf Area Index (LAI) or root depth which may affect simulated transpiration, and uncertainties associated with sap flow measurements (Köstner et al., 1998). While our linear interpolations between the destructive LAI measurements made at about 6 month-intervals led to slow intra-annual variations in LAI, destructive (Christina et al. 2017) and remote sensing measurements (le Maire et al., 2011) made at higher frequencies in nearby *Eucalyptus* plantations showed that seasonal LAI changes can be more rapid. Also, despite specific calibrations of sap flow probes for *E. grandis* trees at our study site, uncertainties might still be associated with sap flow measurements and their extrapolation to the stand. Time series of soil water content down to a depth of 6 m were satisfactorily predicted over stand growth in the 4 treatments, as in a previous study using the MAESPA model in *E. grandis* plantations (Christina et al., 2017).

The depth of the water table is site-dependent and cannot change over short distances in a field experiment of throughfall exclusion. Our objective here was to simulate the water table dynamics that would have occurred in a large commercial plantation, by using the initial water table depth and lateral flow parameters obtained in a large nearby *E. grandis* stand growing on a similar soil type (Christina et al., 2017). Since measured structural and physiological tree parameters are inputs in the MAESPA model, there is no feedback between the simulated soil water balance and tree characteristics (e.g. LAI). Therefore, one potential issue comes from the simulation of water uptake from the simulated water table, whereas the depth of the real water table in the experiment can be different. We argue here that this bias leads to limited errors in the simulations for several reasons:

- 1) the water table depth was measured at depths between 15 m and 17 m over the whole rotation in the experiment, which indicates that the trees did not have access to the water table over the first 3 years after planting (unpublished data). This corresponds to our simulations for all treatments, since we simulate almost no water uptake in the water table the first 3 years, and no water uptake below 14 m.

2) In the 4<sup>th</sup> year, the simulated water table in all treatments except -K+W reached depths similar to the depth measured in the experiment (i.e. 17 m). In these treatments, we simulated water uptake from the water table during that year, which was also probably occurring in the experiment.

3) In -K+W, there was nearly no simulated water uptake in the water table, even though the level of the water table was simulated to be shallower than in the other treatments. This lack of water uptake from the water table is therefore highly probable in the experimental plots where the water table was 6–8 meters deeper than in the simulations. The quantification of the effects of K and water supply regimes on water storage in very deep soil layers as well as deep water seepage, which likely influences stream flows in catchments covered by eucalypt plantations, was among the most interesting outputs of our simulation approach.

#### **4.2. Consequences of contrasting K and water supply regimes on Eucalyptus water use and tree water stress**

In agreement with our first hypothesis, a reduction in rainfall decreased tree water use and the recharge of the water table, and increased tree water stress (shown by  $I_{SWS}$ ) and the depth of water uptake in the soil. The soil-driven tree water stress index is an instantaneous index measuring the impact of the soil water availability on transpiration. Under a saturated soil, many tree traits should be impacted in turn due to plant plasticity (e.g. LAI), which was not the case in our simulation; therefore, the computed index act as an instantaneous water stress index considering only the direct effect of soil water content to stomatal conductance and plant transpiration. A decrease in recharge of the water table after planting in response to a decrease in rainfall led to a drop of the water table level, through the continuous outgoing flow of groundwater within the catchment. A strong effect of the management of eucalypt plantations on the depth of the water table has already been shown in Brazil with a rise from -26 m to -16 m after clearcutting (Almeida et al., 2007). In this experimental catchment covered by highly productive plantations, the deep seepage over an entire rotation amounted to 3.6% of the total precipitation (1147 mm yr<sup>-1</sup> on average), which is consistent with our findings in K-fertilized plots. The contribution of soil water stored in deep soil layers is critical for tree survival in regions with frequent droughts. In Australia, *Eucalyptus* plantations with high stocking densities were highly sensitive to drought after 3 years of growth during dry periods (Harper et al., 2014). A strong relationship between tree growth rates (and mortality) and water table depth has been shown in groundwater-dependent ecosystems (Eamus et al., 2015), and in particular in *Eucalyptus* and *Pinus* forests (McGrath et al., 1991; Harper et al., 2009; Zolfaghar et al. 2016).

In agreement with our second hypothesis, a severe K-deficiency of *E. grandis* trees led to low water use and tree water stress (shown by  $I_{SWS}$ ) in comparison with K-fertilized trees, and enhanced the recharge of the water table. A growing body of evidence suggests that forests are less prone to water deficit under low than under high nutrient availability, as shown for *Eucalyptus* and *Pinus* plantations (Linder et al., 1987; Mendham et al., 2011; White et al., 2009; Battie-Laclau et al., 2014a). Water stress and tree mortality in *Eucalyptus* plantations increased in response to nitrogen fertilization in Australia (Carter and White, 2009; Stoneman et al., 1997).

Increase in tree water stress in response to K fertilization (this study), and N fertilization (White et al., 2009; Mendham et al., 2011) might also occur for other nutrients, when a strong deficiency in the soil is removed by fertilizer addition.

Despite the beneficial effect of nutrient supply on plants resistance to abiotic stresses (Cakmak, 2005; Reddy et al., 2004), our study emphasizes possible drawbacks of high fertilization on tree water stress over dry periods in fast-growing planted forests. The fertilizations greatly increase leaf area and biomass production in *Eucalyptus* plantations (Leuning et al., 1991a; Clearwater and Meinzer, 2001; Epron et al., 2012; Smethurst, 2010; du Toit et al., 2010), as well as photosynthetic activities in expanded leaves (Leuning et al., 1991b; Battie-Laclau et al., 2014b, Forrester et al., 2013). High productivity in these fast-growing plantations is associated with high transpiration rates, which leads to low water storage in deep soil layers during rainy seasons (Christina et al., 2017) and might lead to an increase in tree water stress during the following dry periods.

Our results suggest that an adequate nutrient supply can help mitigate the adverse consequences of low precipitation on tree water stress and soil water resources. We compared highly fertilized trees with severe K deficiency in our study, but intermediate K fertilizer addition should also be studied. Addition of sodium instead of potassium in the K-deficient soil of our study site led to intermediate water stress of *E. grandis* trees (shown by predawn leaf water potential) and wood production between K-fertilized trees and K-deficient trees (Battie-Laclau et al., 2014a).

### **4.3. Managing water in eucalypt plantations under climate changes**

Tropical and subtropical planted forests provided 65% of the global wood consumption in 2012 (Payn et al., 2015). However, the intensity and duration of dry periods will probably increase in the future in many tropical and subtropical regions (Solomon et al., 2009). Therefore, management practices improving tree tolerance to severe drought are needed to satisfy a continuously increasing demand in wood (FAO, 2010). The share between blue and green water is a major issue in many regions (Farley et al., 2005; Jackson et al., 2005; Falkenmark and Rockström, 2006). While low evapotranspiration rates contribute to maintaining stream flows in afforested catchments, high evapotranspiration rates can positively affect the regional climate, though decrease in land-surface temperatures, and increase in atmospheric humidity and precipitations (Bonan, 2008; Peng et al., 2014; Alkama et Cescatti, 2016; Syktus and McAlpine, 2016). Managing water in eucalypt plantations and more generally in agricultural lands is therefore challenging to cope with both local and global issues.

Our study shows that soil depth is an essential criterion to consider for the selection of new afforestation sites in tropical regions prone to severe droughts. The depth of the soil explored by tree roots strongly influences the soil water storage capacity and the amount of water available for tree growth during dry periods (Harper et al., 2014, 2009; Laclau et al., 2013). Even though planting water-resistant genotypes is essential to limit the risks of tree mortality, the most resistant clones are not the most productive. Selecting the genotype to plant in



each plot, forest managers make a compromise between the potential wood production and the risk of mortality during prolonged drought periods. Management practices leading to a reduction in stand transpiration in comparison with intensively managed plantations can contribute to increasing water storage in deep soil layers. Stand water use can be decreased through a reduction in LAI, which can be achieved by lowering stocking rates relative to the most productive plantations (Mendham et al., 2011; Harper et al., 2014). However, tree plasticity leads to an increase in leaf area per tree when the stocking density decreases in *Eucalyptus* plantations (Le Maire et al., 2013; Stoneman et al., 1997), and a sharp decrease in the stocking density is therefore needed to substantially reduce LAI. Moreover, low stocking densities can have some drawbacks for the silviculture in *Eucalyptus* plantations (e.g. more difficulties to control weeds, big trunks to harvest,...) and other management options could be considered to improve the tolerance of tropical plantations to drought. Reducing the rotation length (i.e. the time between two successive harvests) could be another means of reducing tree water stress, with a more frequent recharge of water in deep soil layers after clear cutting. For example, a rise of 6-10 m of the water table after clear cutting followed by a drop down to its initial depth has been observed in commercial eucalypt plantations intensively studied in two Brazilian states (Almeida et al. 2007; Christina et al., 2017). Thinning at mid rotation could also be an alternative to open the canopy and significantly reduce evapotranspiration and tree water stress in the last years before the final harvest (White et al. 2009).

Fertilization regimes can be a flexible tool to improve local trade-offs between wood production and water resources. A reduction in fertilizer supply relative to current practices can strongly decrease stand water use and therefore contribute to enhancing tree tolerance to drought, but at the expense of stand productivity (White et al., 2009; Battie-Laclau et al., 2016, Christina et al., 2015). Fertilization regimes could be associated with other management practices (i.e. rotation length, stocking densities, thinning at mid rotation...) to limit the adverse consequences of severe droughts while maintaining a high wood production. Major changes in management practices would be operationally challenging. High risks of tree mortality in a changing climate might require changes in the productivity objectives of tropical planted forests (Battie-Laclau et al. 2014a; Harper et al. 2014). The marked effect of drought on tree water uptake from deep soil layers in our study also suggests that management practices designed to reduce stand water use (and therefore stand productivity) might also be useful to maintain stream flows in some regions under a future drier climate.

## 5. Conclusion

Fertilization regimes strongly influence tree water use in intensively managed *Eucalyptus* plantations and can be used, among other management options, as a tool to decrease tree water stress through an increase in water storage in deep soil layers during rainy seasons. A decrease in annual rainfall increases the mean soil depth of water withdrawal, decreases the residual soil water content in deep soil layers and leads to a drop of the water table level. The negative impact of a decrease in annual rainfall on soil water resources was lower for K-deficient trees than for K-fertilized trees. Our study suggests that, in a context of climate change, current

levels of nutrient supply in tropical planted forests might be revised to improve tree tolerance to severe droughts and to adjust the partitioning between blue and green waters to face both global and local issues.

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## Supplementary informations

**Table A1. MAESPA parameters constant between treatments. Names, symbols, units, values and sources are presented**

<b>Names and definition</b>	<b>Symbols</b>	<b>Units</b>	<b>Value</b>	<b>Sources</b>
<i>Stomatal conductance parameter</i>				
Minimum stomatal conductance at low photosynthesis	$g_{01}$	$\text{mol m}^{-2} \text{s}^{-1}$	0.021	Christina et al., 2017
Minimum stomatal conductance at high photosynthesis	$g_{02}$	$\text{mol m}^{-2} \text{s}^{-1}$	-0.337	"
Empirical coefficient	$g_{11}$	d.u.	4.675	"
Empirical coefficient	$g_{12}$	d.u.	21.625	"
Sensitivity parameter	$S_f$	d.u.	2.253	"
Bulk leaf water potential	$\psi_f$	MPa	-2.899	"
CO <sub>2</sub> compensation point	$\gamma$	ppm	0.632	"
<i>Canopy storage parameter</i>				
Maximum canopy storage	$S$	mm	0.21	Christina et al., 2017
Canopy drainage parameters	a, b	$\text{mm min}^{-1}$ ; d.u.	0.002, 3.7	"
<i>Other water balance parameters</i>				
Minimum root water potential	$\Psi_{\min}$	MPa	-1.6	Duursma & Medlyn 2012
Gravimetric potential	$\Psi_{\text{grav}}$	MPa $\text{m}^{-1}$	0.01	Duursma et al., 2008
Proportion of lateral drainage	$P_{\text{lat}}$	d.u.	0.00008	Christina et al., 2017
Initial depth of water table		m	18.5	"

**Table A2. MAESPA parameters varying with stand age or treatments used in the study.**

Treatment		+K +W				-K +W				+K -W				-K -W			
Stand age	units	1y	2y	3y	4y	1y	2y	3y	4y	1y	2y	3y	4y	1y	2y	3y	4y
Throughfall exclusion	%	0%	0%	0%	0%	0%	0%	0%	0%	37%	37%	37%	37%	37%	37%	37%	37%
<b>Morphological parameters</b>																	
Leaf area index	m <sup>2</sup> m <sup>-2</sup>	3.35	4.53	5.14	4.30	2.57	2.59	1.88	1.93	3.60	3.94	4.29	3.41	2.48	2.76	2.01	1.89
Tree height	m <sup>2</sup> m <sup>-2</sup>	4.98	10.51	15.48	18.99	3.64	7.27	10.79	12.96	5.22	10.49	14.96	17.44	3.97	7.74	11.44	13.53
Crown diameter	m <sup>2</sup> m <sup>-2</sup>	3.0	3.3	3.5	3.5	2.7	3.2	3.5	3.4	2.9	3.2	3.4	3.4	2.7	3.0	3.2	3.3
Leaf inclination angle	°	28.2	45.5	48.9		24.2	34.9	41.5		32.4	47.5	50		29.6	41.5	42.3	
<b>Physiological parameters</b>																	
J <sub>MAX</sub>	μmol m <sup>-2</sup> s <sup>-1</sup>		142.8	166.3			108.3	130.5			142.1	124.5			121.1	116.4	
V <sub>C</sub> MAX	μmol m <sup>-2</sup> s <sup>-1</sup>		45.9	91.8			50.3	62.8			63.2	70.8			45.6	50.4	
R <sub>d</sub>	μmol m <sup>-2</sup> s <sup>-1</sup>		1.32	2.91			1.45	2.65			1.82	2.24			1.17	1.71	
Quantum yield	mol e <sup>-</sup> mol <sup>-1</sup> aPAR			0.354				0.307				0.288				0.361	
Plant conductance	mmol m <sup>-2</sup> s <sup>-1</sup> MPa <sup>-1</sup>		0.92	1.33			0.58	1.43			0.88	1.93			0.73	1.59	
<b>Root parameters</b>																	
Fine root mass density	g m <sup>-2</sup>	297	388.6	898.5		197	253.9	695.8		185	427.1	960.4		141	278.4	597.7	
Root radius	mm		0.394	0.513			0.372	0.458			0.349	0.525			0.349	0.450	
Specific root length	m g <sup>-1</sup>		26.73	19.82			33.11	20.48			29.53	18.45			29.49	21.22	
<b>Maximum rooting depth parameters</b>																	
a	m			16.61				16.61				19.05					15.96
b	day <sup>-1</sup>			0.00202				0.00202				0.00207					0.00203
c	d.u.			1.5883				1.5883				1.8394					1.5424
source		Christina et al., 2015		This study		Christina et al., 2015		This study		Christina et al., 2015		This study		Christina et al., 2015		This study	



**Table A3. Soil retention parameters and conductivity. Minimum soil water is presented for each treatment.**

Soil retention parameters and conductivity										
Minimum soil water content for root absorption ( $\theta_v$ )										
Depth (m)	+K+W	-K+W	+K-W	-K-W	$\alpha_\psi$	$\theta_{VS}$	n	$K_{SAT}$	$\theta_l$	$\theta_R$
0-0.33	0.0843	0.0853	0.0638	0.0733	1000	0.355	1.73	751.4	0.355	0.0638
0.33 - 0.66	0.0769	0.081	0.0605	0.0725	3823	0.322	1.72	892.6	0.322	0.0605
0.66 - 1	0.0757	0.0818	0.0619	0.0752	701	0.317	1.69	781.7	0.317	0.0619
1 - 1.5	0.0842	0.0898	0.0694	0.0819	625	0.317	1.79	642.8	0.317	0.0694
1.5 - 2	0.0923	0.0997	0.0763	0.0919	519	0.323	1.95	462.5	0.323	0.0763
2 - 2.5	0.0999	0.1116	0.0826	0.1054	396	0.334	2.14	268.3	0.334	0.0826
2.5 - 3	0.1075	0.1235	0.0889	0.1188	316	0.340	2.19	112.9	0.340	0.0889
3 - 3.5	0.1136	0.133	0.0948	0.1291	"	"	"	107.3	"	0.0948
3.5 - 4	0.1183	0.1403	0.1004	0.1362	"	"	"	101.6	"	0.1004
4 - 4.5	0.123	0.1476	0.106	0.1434	"	"	"	96.0	"	0.106
4.5 - 5	0.1292	0.1563	0.112	0.1501	"	"	"	90.4	"	0.112
5 - 5.5	0.1372	0.1666	0.1184	0.1562	"	"	"	84.8	"	0.1184
5.5 - 6	0.145	0.1769	0.1248	0.1624	"	"	"	79.2	"	0.1248
6 - 6.5	0.145	0.1706	0.1316	0.1598	"	"	"	68.5	"	0.1316
6.5 - 7	0.1473	0.1643	0.1383	0.1571	"	"	"	58.9	"	0.1383
7 - 7.5	0.1495	0.1581	0.145	0.1545	"	"	"	"	"	0.145
7.5 - 8	0.158-0.19	0.158-0.19	0.158-0.19	0.158-0.19	"	"	"	"	"	0.15-0.19
Source	Christina et al., 2015 and extrapolation					Christina et al., 2017				This study

**Table A4. Fraction of root per each layer in the different treatment, data from Christina et al., 2015.**

Depth (m)	Fraction of root biomass in each layer( $R_{Dis}$ )							
	+K+W		-K+W		+K-W		-K-W	
	24 months	36 months	24 months	36 months	24 months	36 months	24 months	36 months
0-0.33	0.16658	0.14025	0.26028	0.20913	0.19364	0.20814	0.20710	0.23022
0.33 - 0.66	0.10257	0.07352	0.15283	0.11603	0.10480	0.08135	0.11476	0.13726
0.66 - 1	0.17795	0.09221	0.12461	0.12326	0.15141	0.12601	0.19844	0.13938
1 - 1.5	0.09805	0.04705	0.12776	0.06893	0.07014	0.06679	0.09335	0.07133
1.5 - 2	0.09805	0.04705	0.12776	0.06893	0.07014	0.06679	0.09335	0.07133
2 - 2.5	0.06632	0.05791	0.06128	0.05601	0.05405	0.05004	0.03860	0.04214
2.5 - 3	0.06632	0.05791	0.06128	0.05601	0.05405	0.05004	0.03860	0.04214
3 - 3.5	0.01751	0.03472	0.01979	0.02203	0.03229	0.03311	0.04547	0.01664
3.5 - 4	0.01751	0.03472	0.01979	0.02203	0.03229	0.03311	0.04547	0.01664
4 - 4.5	0.03188	0.05119	0.00932	0.03625	0.03197	0.03925	0.01868	0.05399
4.5 - 5	0.03188	0.05119	0.00932	0.03625	0.03197	0.03925	0.01868	0.05399
5 - 5.5	0.01730	0.04169	0.00609	0.03051	0.04309	0.01341	0.01123	0.03591
5.5 - 6	0.01730	0.04169	0.00609	0.03051	0.04309	0.01341	0.01123	0.03591
6 - 6.5	0.00986	0.04856	0.00194	0.01526	0.01335	0.02234	0.00427	0.00829
6.5 - 7	0.00986	0.04856	0.00194	0.01526	0.01335	0.02234	0.00427	0.00829
7 - 7.5	0.01723	0.01998	0.00452	0.02086	0.01719	0.02481	0.01613	0.01297
7.5 - 8	0.01723	0.01998	0.00452	0.02086	0.01719	0.02481	0.01613	0.01297
8 - 8.5	0.01148	0.01475	0.00029	0.00708	0.00804	0.01791	0.01149	0.00375
8.5 - 9	0.01148	0.01475	0.00029	0.00708	0.00804	0.01791	0.01149	0.00375
9 - 9.5	0.00402	0.00812	0.00006	0.00084	0.00437	0.01386	0.00006	0.00122
9.5 - 10	0.00402	0.00812	0.00006	0.00084	0.00437	0.01386	0.00006	0.00122
10 - 10.5	0.00003	0.01458	0.00005	0.00517	0.00037	0.00427	0.00046	0.00018
10.5 - 11	0.00003	0.01458	0.00005	0.00517	0.00037	0.00427	0.00046	0.00018
11 - 11.5	0.00276	0.00288	0.00004	0.00493	0.00023	0.00441	0.00009	0.00003
11.5 - 12	0.00276	0.00288	0.00004	0.00493	0.00023	0.00441	0.00009	0.00003
12 - 12.5	0	0.00206	0	0.00301	0	0.00180	0	0.00003
12.5 - 13	"	0.00206	"	0.00301	"	0.00180	"	0.00003
13 - 13.5	"	0.00024	"	0.00260	"	0.00003	"	0.00003
13.5 - 14	"	0.00024	"	0.00260	"	0.00003	"	0.00003
14 - 14.5	"	0.00201	"	0.00118	"	0.00015	"	0.00002
14.5 - 15	"	0.00201	"	0.00118	"	0.00015	"	0.00002
15 - 15.5	"	0.00052	"	0.00055	"	0.00002	"	0
15.5 - 16	"	0.00052	"	0.00055	"	0.00002	"	"
16-16.5	"	0	"	0	"	0.00002	"	"
16.5-17	"	"	"	"	"	0.00002	"	"



## **Simulation de pratiques de gestion alternatives pour l'adaptation des plantations pérennes aux changements globaux**

Dans le cadre de cette thèse, nous avons utilisé deux modèles mathématiques complémentaires pour simuler le comportement futur des plantations de café sous conditions actuelles ainsi que sous changements climatiques (1979 -2100). Nous avons étudié leurs bilans de carbone, d'eau et d'énergie pour mieux comprendre et prévoir les effets des changements sur la production de café. Comparativement à une plantation en plein soleil, l'ajout d'arbres d'ombrage au dessus des caféiers pourrait permettre d'augmenter les rendements lorsque la température augmente. Cependant, les rendements en grain de caféiers à l'horizon 2100 sont prédits inférieurs aux rendements actuels quelle que soit l'espèce d'arbres d'ombrage ou sa gestion.

**Mots-clés : MAESPA, écophysiologie, café, eucalyptus, agroforesterie, modélisation, changements climatiques**

## **Simulation of alternative management practices for perennial plantations adaptation to global changes**

In this thesis, we used two complementary mathematical models to simulate the future behavior of coffee plantations under climate change (1979 - 2100). We studied their carbon, water, and energy balances to better understand and predict the effects of these changes on coffee production. The addition of shade trees above the coffee layer lead to higher yield compared to full sun management under increased temperature. However, coffee yield was predicted to decrease compared to current levels by 2100, whatever the shade tree species or management.

**Keywords: MAESPA, ecophysiology, coffee, eucalyptus, agroforestry, modelling, climate change**