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# Modeling radiative transfer of Sun-Induced Fluorescence, thermal emission and radiative budget of 3D vegetation canopies: towards a comprehensive 3D SIF model

Omar Regaieg

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# THÈSE

En vue de l'obtention du  
**DOCTORAT DE L'UNIVERSITÉ DE TOULOUSE**  
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---

Présentée et soutenue par  
**Omar REGAIEG**

Le 12 janvier 2023

**Modélisation du transfert radiatif de la fluorescence induite par le soleil, de l'émission thermique et du bilan radiatif des couverts végétaux 3D : vers un modèle SIF complet**

---

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Modeling Radiative Transfer of Solar-Induced Fluorescence,  
Thermal Emission and Radiative Budget of 3D Vegetation  
Canopies: Towards a Comprehensive 3D SIF Model

by

Omar REGAIEG (عمر الرقيّو)

A thesis submitted for the degree of

*Doctor of Philosophy*

2023



*“In the darkness, all the ordinary colors of our daylight world disappear. Only the intensely glowing hues of fluorescent substances touched by the ultraviolet beam shine out with striking clarity.”*

Sterling Gleason, 1960

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# List of publications

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4. Wang, Y., Kallel, A., Yang, X., **Regaieg, O.**, Lauret, N., Guilleux, J., Chavanon, E., & Gastellu-Etchegorry, J.-P. (2022). DART-Lux: An unbiased and rapid Monte Carlo radiative transfer method for simulating remote sensing images. *Remote Sensing of Environment*, 274, 112973. <https://doi.org/10.1016/j.rse.2022.112973>

5. Yang, X., Wang, Y., Yin, T., Wang, C., Lauret, N., **Regaieg, O.**, Xi, X., & Gastellu-Etchegorry, J. P. (2022). Comprehensive LiDAR simulation with efficient physically-based DART-Lux model (I): Theory, novelty, and consistency validation. *Remote Sensing of Environment*, 272, 112952. <https://doi.org/10.1016/j.rse.2022.112952>

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# Abstract

The photosynthetic activity of vegetation is of major interest given current environmental concerns such as climate change and water resources. In this process, chlorophyll molecules excited by absorption of photosynthetically active radiation (PAR), dissipate some of the energy not used for photosynthesis in the form of heat and fluorescence radiation (SIF) which turns out to be a reliable and instantaneous indicator of photosynthetic activity. However, many factors complicate the interpretation of remote sensing measurements in terms of SIF and thus photosynthetic activity. In particular, the 3D architecture of the vegetation greatly affects radiation propagation, and thus PAR absorption, SIF emission in the canopy, and the remote sensing measurement. Accurate modeling of SIF emission and remote sensing measurements is therefore essential to accurately interpret these measurements in terms of SIF emitted (*i.e.*, photosynthetic activity) by the vegetation. Moreover, it must be adapted to complex landscapes of large dimensions, at least larger than the resolution of the relevant satellite sensors (*e.g.*, 300 m for the upcoming ESA FLEX satellite mission to measure SIF). Given the number, complexity and diversity of terms to be taken into account, this modeling uses strong approximations that often lead to significant errors in the interpretation of remote sensing measurements. The model developed in this thesis deals mainly with the radiative aspect. It is based on the DART radiative transfer model (<https://dart.omp.eu>). Based on the discrete ordinate method, DART-FT, the initial mode of DART, simulates the SIF emission and the remotely sensed SIF signal, but has computational requirements (*i.e.*, memory, computational time) that are prohibitive for the simulation of large landscapes. The new mode of DART, called DART-Lux, solves this problem with a very efficient two-way Monte Carlo algorithm. To complement the functionality of DART-Lux, four original models have been designed and implemented. (1) Modeling of landscapes with turbid volumes and facets, as the "turbid" representation is often useful for simulating large landscapes. (2) Modeling of SIF emission and the SIF signal that is measured by satellite, airborne and in-situ sensors. It takes into account local bioclimatic conditions via a coupling with the SCOPE energy balance model. Applied to



eight forest plots realistically reconstructed with LiDAR measurements, this modeling allowed one to study the impact of the 3D structure of the vegetation on the SIF emission and on the SIF observed by a sensor at nadir, from morning to evening. It highlighted that the relative error made by neglecting the 3D architecture of the canopies, as in the 1D models, is often greater than 30%, especially in the morning and evening when the solar direction is very oblique. (3) Modeling of remote sensing images corresponding to the thermal emission of the landscape. As DART is not an energy balance model, the 3D temperature distribution is imported or approximated via short-wave illumination. (4) 3D radiation balance modeling with the ability to simulate it by sub-scene and feature type. All of these modeling, with the exception of the radiation balance modeling, were found to be very accurate and efficient in terms of computation time and memory volume, with gains often greater than 100. The resulting new DART model opens very interesting perspectives for the study of land surfaces using remote sensing observations in the visible to thermal infrared range. This work is currently being pursued in order to take into account the multiple biophysical interactions within the canopies that condition their SIF emission and their 3D temperature.

# Résumé

L'activité photosynthétique de la végétation revêt un intérêt majeur compte tenu des préoccupations environnementales actuelles comme le changement climatique et les ressources en eau. Dans ce processus, les molécules de chlorophylle excitées par absorption de rayonnement photosynthétiquement actif (PAR), dissipent une part de l'énergie non utilisée pour la photosynthèse sous forme de chaleur et de rayonnement de fluorescence (SIF) qui ainsi est un indicateur fiable et instantané de l'activité photosynthétique. Cependant, de nombreux facteurs compliquent l'interprétation des mesures de télédétection en termes de SIF et donc d'activité photosynthétique. En particulier, l'architecture 3D de la végétation affecte beaucoup la propagation du rayonnement, et donc l'absorption du PAR, l'émission de SIF dans le couvert végétal, et la mesure de télédétection. Une modélisation précise de l'émission SIF et des mesures de télédétection est donc essentielle pour interpréter avec précision ces mesures en termes de SIF émis (i.e., activité photosynthétique) par la végétation. De plus, elle doit être adaptée aux paysages complexes de grandes dimensions, du moins plus grands que la résolution des capteurs satellites concernés (e.g., 300 m pour la prochaine mission satellite FLEX de l'ESA pour mesurer la SIF). Vu le nombre, complexité et diversité des termes à prendre en compte, cette modélisation utilise de fortes approximations qui induisent souvent de grandes erreurs lors de l'interprétation des mesures de télédétection. La modélisation développée dans cette thèse traite principalement de l'aspect radiatif. Elle s'appuie sur le modèle de transfert radiatif DART (<https://dart.omp.eu>). Le mode initial, DART-FT, de DART, basé sur la méthode des ordonnées discrètes, simule l'émission SIF et le signal SIF mesuré par télédétection, mais a des besoins informatiques (i.e., volume mémoire, temps de calcul) prohibitifs pour simuler de grands paysages. Le nouveau mode, appelé DART-Lux, résout ce problème via un algorithme bidirectionnel Monte Carlo très efficace. Pour compléter les fonctionnalités de DART-Lux, quatre modélisations originales ont été conçues et implémentées. (1) Modélisation de paysages avec des volumes turbides et des facettes, car la représentation "turbide" est souvent utile pour simuler de grands paysages. (2) Modélisation de l'émission et mesure satellite de la SIF, en

tenant compte des conditions bioclimatiques locales via le couplage avec le modèle de bilan d'énergie SCOPE. A partir de huit parcelles forestières reconstruites de manière réaliste avec des mesures LiDAR, cette modélisation a permis d'étudier l'impact de la structure 3D de la végétation sur la SIF émise et observée par un capteur au nadir, du matin au soir. Ainsi, l'erreur relative commise en négligeant l'architecture 3D des couverts, comme dans les modèles 1D, est souvent supérieure à 30%, surtout les matins et soirs quand la direction solaire est très oblique.

(3) Modélisation des images de télédétection correspondant à l'émission thermique du paysage. DART n'étant pas un modèle de bilan d'énergie, la distribution 3D des températures est importée ou calculée de manière approchée via un éclairage dans les courtes longueurs d'onde.

(4) Modélisation du bilan radiatif 3D avec possibilité de le simuler par sous scène et par type d'élément. Toutes ces modélisations, excepté la modélisation du bilan radiatif, se sont avérées très précises et efficaces en termes de temps de calcul et de volume mémoire, avec des gains souvent supérieurs à 100. La modélisation implémentée dans DART ouvre donc des perspectives très intéressantes pour l'étude des surfaces terrestres avec l'aide d'observations de télédétection visible à infrarouge thermique. Ce travail est actuellement poursuivi, pour tenir compte des multiples interactions biophysiques qui au sein des couverts conditionnent leur émission SIF et température 3D.

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# General introduction

Photosynthesis is a biochemical process consisting in transforming carbon dioxide (CO<sub>2</sub>) molecules captured from the atmosphere and water molecules absorbed from the soil into carbohydrates and dioxygen molecules by green vegetation. This endothermic reaction uses the solar radiation as a source of energy. It is a fateful process for the human kind and for life on Earth in general. Indeed, it is the main process used by primary producer organisms to produce organic compounds necessary to provide energy to all the elements of the food chain. Moreover, it plays a crucial role in the carbon cycle on Earth as it makes green vegetation work as a carbon sink that uptakes atmospheric CO<sub>2</sub> released by natural phenomena (*e.g.*, respiration of living organisms, fires, etc.) and especially by anthropogenic activities (*e.g.*, industrial activities, fossil fuels burning, etc.), then to store it as biomass. Therefore, it reduces the impact of human carbon footprint on the atmospheric CO<sub>2</sub> concentration which continues to increase at an alarming rate since the 19<sup>th</sup> century. The global warming and climate change, caused by greenhouse gases including CO<sub>2</sub> that prevent the heat received by the Earth surface through the sun radiation from escaping to external space, are seriously impacting and even threatening human life. They are causing an increase in the average temperature of the planet and in the frequency of extreme weather events such as droughts (Cogato et al., 2019) and thus are becoming major concerns for contemporary human societies. Furthermore, the world population is increasing and therefore there is an increasing demand on food that needs to be satisfied. Consequently, in the recent years, the scientific community has become increasingly interested in studying the photosynthetic process at different spatial and temporal scales, both for agricultural and forest canopies, in order address these urgent and critical challenges of humanity.

Earth surfaces emit and scatter electromagnetic radiation over the entire spectrum, with differences depending on the spectral domain (*e.g.*, optical and microwave domains). The measurement of this radiation by active and passive remote sensing can provide information on

the characteristics of these surfaces. In particular, multispectral and hyperspectral optical sensors onboard Earth observation satellites are very useful for large scale vegetation monitoring. Indeed, they provide high spatial and temporal resolution observations in different spectral domains (*e.g.*, visible, near-infrared, thermal infrared) used for inferring biophysical and biochemical information about vegetation (*e.g.*, LAI, biomass, chlorophyll content, water content, etc.). However, they generally cannot provide real-time information on the photosynthetic process of vegetation, which is essential for detecting eventual stresses, and in particular water and temperature stress. For instance, retrieved information such as current pigments content (*e.g.*, chlorophyll, carotenoid) of vegetation generally results from past bioclimatological conditions (*e.g.*, photosynthesis inhibited by water or temperature stress) that influence vegetation optical properties sometime later, when these changes can be irreversible. Presently, only two types of remote sensing measurements can provide real-time information on plant responses to stress. 1) Reflection of sun radiation at 0.531  $\mu\text{m}$  and 0.570  $\mu\text{m}$ , used to define the photochemical reflectance index (PRI), can indicate short-term changes in the xanthophyll cycle (Gerhards et al., 2019; Suárez et al., 2009). 2) Thermally emitted radiation can indicate changes in temperature that can allow early stress detection (Costa et al., 2013; Gerhards et al., 2019).

Solar-induced chlorophyll fluorescence (SIF) is a spontaneous re-emission of radiation by vegetation excited by photosynthetically active solar radiation. Together with the photochemical and heat dissipation processes, they form the three possible ways for an excited chlorophyll molecule to dispose of the excess of energy. These three processes are in competition, which makes the SIF correlated with photosynthetic activity and gross primary production. Because its response to the inhibition of photosynthesis due to stress is instantaneous, SIF is a real-time indicator of the photosynthetic process, and therefore a potentially very useful signal for monitoring the vegetation functioning state and for stress detection.

SIF represents a small fraction of the sun radiation scattered by vegetation and it is spectrally overlapping with it. Hence, except for some absorption bands (*e.g.*, atmospheric oxygen O<sub>2</sub>A and O<sub>2</sub>B absorption bands, Fraunhofer lines of solar radiation), it is impossible to dissociate it from the total radiation outgoing from the vegetation at the top of canopy (TOC) or at the top of atmosphere (TOA) levels. Indeed, in these absorption bands, the solar incident radiation and therefore the scattered radiation are small enough such that the SIF can be detected and

measured. We usually observe small peaks of the TOC reflectance spectrum at these bands. This is explained by the fact that the radiation absorbed at a given wavelength gives rise to fluorescence at other wavelengths, and therefore increases the apparent reflectance at these bands. In recent years, many techniques for retrieving the SIF signal from in-situ, airborne and spaceborne sensors within the oxygen O<sub>2</sub>A and O<sub>2</sub>B absorption bands and the Fraunhofer lines were developed. The European Space Agency (ESA) has shown a particular interest in SIF and its potential to monitor vegetation functioning from space using these techniques and has selected the Fluorescence Explorer (FLEX) satellite as its eighth Earth Explorer mission.

Nevertheless, the interpretation of SIF measurements remains challenging. Indeed, although the atmospheric oxygen allows to measure the SIF because it attenuates the incident radiation, it also attenuates the SIF signal before reaching the sensor especially for spaceborne sensors. Therefore, accurate atmospheric corrections are needed to retrieve the TOC signal. Moreover, TOC SIF directly measured by TOC sensors or retrieved from TOA sensors is solely a part of the total SIF emitted within the canopy that escapes from it, directly or after being scattered, to the observation direction. Most of the SIF radiation escapes to other directions, or is absorbed by the canopy elements (*e.g.*, leaves, woody elements, soil, etc.). Besides, in addition to the instantaneous photosynthetic activity, the SIF measurements are influenced by several other confounding factors, such as the photosynthetically active radiation absorption, the canopy structure, the optical properties of canopy elements, the sun-canopy-sensor configuration, etc.

For these reasons, models that simulate SIF emission and observations stand out as essential tools to help in retrieving and interpreting the SIF signals from measurements and to disentangle the effect of each influencing factor. Ideally, these models should take into account all the parameters that affect the SIF emission and observation including the local climatological conditions that affect the temperature dependent photosynthetic rate and therefore the leaf-level SIF emission, the canopy's 3D structure and optical properties and the experimental configurations that affect the radiation propagation. Hence, the full energy balance should be simulated including all the radiative and non-radiative processes with an accurate 3D representation of the canopy. Radiative energy exchanges include the absorption of solar radiation and the emission of thermal radiation, while non-radiative energy exchanges include sensible and latent heat exchanges with the atmosphere and the soil.

Currently, the canopy SIF models developed by the scientific community can be classified into two major groups: 1) 1D models that simulate the full energy balance by taking into account all the major physical processes that cause SIF emission. They include a leaf-level photosynthesis model and a 1D radiation canopy model. However, they neglect the 3D architecture of canopies. The reference models are SCOPE and its multilayer version mSCOPE. 2) 3D radiative transfer models that accurately simulate the propagation of radiation within the canopy. They also include a leaf-level SIF model. However, they do not simulate the non-radiative processes. Among these models, the Discrete Anisotropic Radiative Transfer (DART) model is one of the most comprehensive 3D radiative transfer models. It is developed by CESBIO since 1992. It includes the Fluspect leaf SIF model and therefore simulates canopy SIF emission as well as TOC and TOA SIF observations since 2017. Its initial version, DART-FT, is based on an adapted discrete ordinates method. A more efficient Monte Carlo based mode, called DART-Lux, has been developed since 2018 for simulating remote sensing images. An initial objective was to include all the functionalities of the DART-FT mode. The approach is not straightforward because DART-Lux uses a modeling approach very different from that of DART-FT.

DART simulates any type of urban or natural landscapes. It can simulate vegetation canopies represented using imported realistic 3D objects, schematic 3D objects created internally by DART or canopies represented using 3D turbid medium. In this thesis, the modeling implementations, including SIF emission, are introduced and tested for the two DART modes (*i.e.*, DART-FT and DART-Lux) and for the two vegetation representation methods (facets, turbid). The SIF introduction in DART allowed to evaluate the impact of 3D structure on a deciduous forest's SIF, using a realistic forest scene reconstructed from LiDAR data. Moreover, the thermal emission and the radiation budget are two important components of the energy budget that quantify the energy exchange of vegetation through radiation. They need to be accurately simulated before the consideration of the energy exchange via non-radiative processes. In this thesis, we also introduce the modeling of thermal emission and radiative budget in DART-Lux. The aim of this work is to provide radiative transfer building blocks towards the development of a comprehensive 3D SIF model.

This thesis is organized in five chapters:

Chapter 1 is an introductory chapter that presents general theoretical concepts about fluorescence, solar-induced fluorescence and its use for monitoring vegetation functioning with remote sensing. It also presents the DART model with a special focus on DART-Lux which will be the most considered in the following chapters.

Chapter 2 presents the SIF modeling in DART-FT for vegetation simulated as facets and as 3D turbid medium.

Chapter 3 presents the SIF modeling in DART-Lux for vegetation simulated as facets and as 3D turbid medium. A novel method was developed to introduce the SIF emission for the bi-directional path tracing. Moreover, the turbid vegetation was introduced in DART-Lux including SIF emission.

Chapter 4 shows the impact of vegetation structure on both the SIF emission and observation. The work is a theoretical study with LiDAR reconstructed forest scenes.

Chapter 5 presents the modeling of the thermal emission and radiative budget in DART-Lux for scene elements simulated as facets and as volumes (turbid medium, fluids).



## *GENERAL INTRODUCTION*

# Introduction générale

La photosynthèse est un processus biochimique consistant à transformer les molécules de dioxyde de carbone ( $\text{CO}_2$ ) captées de l'atmosphère et les molécules d'eau absorbées du sol en hydrates de carbone et en molécules de dioxygène par la végétation verte. Cette réaction endothermique utilise le rayonnement solaire comme source d'énergie. Il s'agit d'un processus fatidique pour l'espèce humaine et pour la vie sur Terre en général. En effet, il s'agit du principal processus utilisé par les organismes producteurs primaires pour produire les composés organiques nécessaires pour fournir de l'énergie à tous les éléments de la chaîne alimentaire. En outre, il joue un rôle crucial dans le cycle du carbone sur Terre, car il permet à la végétation verte de fonctionner comme un puits de carbone qui absorbe le  $\text{CO}_2$  atmosphérique libéré par des phénomènes naturels (*e.g.*, la respiration des organismes vivants, les incendies, etc.) et surtout par les activités anthropiques (*e.g.*, les activités industrielles, la combustion des hydrocarbures fossiles, etc.). Il réduit donc l'impact de l'empreinte carbone humaine sur la concentration de  $\text{CO}_2$  dans l'atmosphère, qui continue d'augmenter à un rythme alarmant depuis le XIX<sup>e</sup> siècle. Le réchauffement de la planète et le changement climatique, causés par les gaz à effet de serre, dont le  $\text{CO}_2$ , qui empêchent la chaleur reçue par la surface de la Terre par le biais du rayonnement solaire de s'échapper vers l'espace extérieur, ont un impact sérieux, voire menaçant sur la vie humaine. Ils provoquent une augmentation de la température moyenne de la planète et de la fréquence des événements climatiques extrêmes tels que les sécheresses (Cogato et al., 2019) et deviennent ainsi des préoccupations majeures pour les sociétés humaines contemporaines. En outre, la population mondiale augmente et il y a donc une demande croissante de produits alimentaires qui doit être satisfaite. Par conséquent, au cours des dernières années, la communauté scientifique s'intéresse de plus en plus à l'étude du processus de photosynthèse à différentes échelles spatiales et temporelles, pour les canopées agricoles et forestières, afin de répondre à ces défis urgents et critiques de l'humanité.

Les surfaces terrestres émettent et diffusent du rayonnement électromagnétique sur l'ensemble du spectre, avec des différences en fonction du domaine spectral (*e.g.*, les domaines optique et micro-ondes). La mesure de ce rayonnement par télédétection active et passive peut fournir des informations sur les caractéristiques de ces surfaces. En particulier, les capteurs optiques multispectraux et hyperspectraux à bord des satellites d'observation de la Terre sont très utiles pour le suivi de la végétation à grande échelle. En effet, ils fournissent des observations à haute résolution spatiale et temporelle dans différents domaines spectraux (*e.g.*, visible, proche infrarouge, infrarouge thermique) utilisées pour déduire des informations biophysiques et biochimiques sur la végétation (*e.g.*, LAI, biomasse, teneur en chlorophylle, teneur en eau, etc.). Cependant, ils ne peuvent généralement pas fournir d'informations en temps réel sur le processus photosynthétique de la végétation, ce qui est essentiel pour détecter d'éventuels stress, et en particulier les stress hydriques et thermiques. Par exemple, les informations récupérées telles que la teneur actuelle en pigments (*e.g.*, chlorophylle, caroténoïde) de la végétation résultent généralement de conditions bioclimatologiques passées (*e.g.*, photosynthèse inhibée par un stress hydrique ou thermique) qui influencent les propriétés optiques de la végétation quelque temps plus tard, lorsque ces changements peuvent être irréversibles. Actuellement, seuls deux types de mesures de télédétection peuvent fournir des informations en temps réel sur les réponses des plantes au stress. 1) La réflexion du rayonnement solaire à 0,531  $\mu\text{m}$  et 0,570  $\mu\text{m}$ , utilisée pour définir l'indice de réflectance photochimique (PRI), peut indiquer des changements à court terme dans le cycle des xanthophylles (Gerhards et al., 2019; Suárez et al., 2009). 2) Le rayonnement émis thermiquement peut indiquer des changements de température qui peuvent permettre une détection précoce du stress (Costa et al., 2013; Gerhards et al., 2019).

La fluorescence chlorophyllienne induite par le soleil (SIF) est une réémission spontanée de rayonnement par la végétation excitée par le rayonnement solaire photosynthétiquement actif. Avec les processus photochimique et de dissipation de chaleur, ils constituent les trois moyens possibles pour une molécule de chlorophylle excitée de se débarrasser de l'excès d'énergie. Ces trois processus sont en compétition, ce qui fait que la SIF est corrélée à l'activité photosynthétique et à la production primaire brute. Parce que sa réponse à l'inhibition de la photosynthèse due au stress est instantanée, la SIF est un indicateur en temps réel du processus photosynthétique, et donc un signal potentiellement très utile pour suivre l'état de fonctionnement de la végétation et pour la détection du stress.

La SIF représente une petite fraction du rayonnement solaire diffusé par la végétation et elle se chevauche spectralement avec celui-ci. Par conséquent, à l'exception de certaines bandes d'absorption (*e.g.*, les bandes d'absorption O<sub>2</sub>A et O<sub>2</sub>B de l'oxygène atmosphérique, les lignes de Fraunhofer du rayonnement solaire), il est impossible de la dissocier du rayonnement total sortant de la végétation en haut de la canopée (TOC) végétale ou en haut de l'atmosphère (TOA). En effet, dans ces bandes d'absorption, le rayonnement solaire incident et donc le rayonnement diffusé sont suffisamment faibles pour que la SIF puisse être détectée et mesurée. On observe généralement des petits pics du spectre de réflectance TOC dans ces bandes. Cela s'explique par le fait que le rayonnement absorbé à une longueur d'onde donnée donne lieu à une fluorescence à d'autres longueurs d'onde, et augmente donc la réflectance apparente à ces bandes. Ces dernières années, de nombreuses techniques ont été développées pour récupérer le signal SIF à partir de capteurs in situ, aéroportés et spatiaux dans les bandes d'absorption de l'oxygène O<sub>2</sub>A et O<sub>2</sub>B et dans les lignes de Fraunhofer. L'Agence Spatiale Européenne (ESA) a montré un intérêt particulier pour la SIF et son potentiel pour suivre le fonctionnement de la végétation depuis l'espace à l'aide de ces techniques et a choisi le satellite Fluorescence Explorer (FLEX) comme sa huitième mission d'observation de la Terre.

Néanmoins, l'interprétation des mesures de la SIF reste difficile. En effet, bien que l'oxygène atmosphérique permette de mesurer la SIF car il atténue le rayonnement incident, il atténue également le signal SIF avant d'atteindre le capteur, surtout pour les capteurs spatiaux. Par conséquent, des corrections atmosphériques précises sont nécessaires pour récupérer le signal TOC. De plus, le signal SIF en TOC directement mesuré par les capteurs TOC ou déduit à partir des capteurs TOA ne représente qu'une partie du signal SIF total émis à l'intérieur de la canopée, qui s'en échappe, directement ou après avoir été diffusé, vers la direction d'observation. La plupart du rayonnement SIF s'échappe vers d'autres directions, ou est absorbé par les éléments de la canopée (*e.g.*, feuilles, éléments ligneux, sol, etc.). En outre, en plus de l'activité photosynthétique instantanée, les mesures de la SIF sont influencées par plusieurs autres facteurs de confusion, tels que l'absorption du rayonnement photosynthétiquement actif, la structure de la canopée, les propriétés optiques des éléments de la canopée, la configuration soleil-canopée-capteur, etc.

Pour ces raisons, les modèles qui simulent l'émission et les observations de la SIF sont des outils essentiels pour aider à récupérer et à interpréter les signaux SIF à partir des mesures et pour démêler l'effet de chaque facteur d'influence. Idéalement, ces modèles devraient prendre

en compte tous les paramètres qui affectent l'émission et l'observation de la SIF, y compris les conditions climatologiques locales qui affectent le taux de photosynthèse dépendant de la température et donc l'émission de la SIF au niveau des feuilles, la structure 3D et les propriétés optiques de la canopée et les configurations expérimentales qui affectent la propagation du rayonnement. Par conséquent, le bilan énergétique complet doit être simulé, y compris tous les processus radiatifs et non radiatifs, avec une représentation 3D précise de la canopée. Les échanges d'énergie radiative comprennent l'absorption du rayonnement solaire et l'émission de rayonnement thermique, tandis que les échanges d'énergie non radiative comprennent les échanges de chaleur sensible et latente avec l'atmosphère et le sol.

Actuellement, les modèles de SIF de canopée développés par la communauté scientifique peuvent être classés en deux groupes principaux : 1) les modèles 1D qui simulent le bilan énergétique complet en prenant en compte tous les processus physiques majeurs qui causent l'émission de la SIF. Ils comprennent des modèles de photosynthèse et de SIF au niveau des feuilles. Cependant, ils négligent l'architecture 3D des canopées. Les modèles de référence sont SCOPE et sa version multicouche mSCOPE. 2) Les modèles de transfert radiatif 3D qui simulent avec précision la propagation du rayonnement dans la canopée. Ils comportent un modèle de SIF au niveau des feuilles. Cependant, ils ne simulent pas les processus non radiatifs. Parmi ces modèles, le modèle de Transfert Radiatif Anisotrope Discret (DART) est l'un des modèles de transfert radiatif 3D les plus complets. Il est développé par le CESBIO depuis 1992. Il inclut le modèle SIF foliaire Fluspect et simule donc l'émission SIF de la canopée ainsi que les observations SIF TOC et TOA depuis 2017. Sa version initiale, DART-FT, est basée sur une méthode adaptée des ordonnées discrètes. Un mode plus efficace basé sur la méthode Monte Carlo, appelé DART-Lux, a été développé depuis 2018 pour simuler les images de télédétection. Un objectif initial était d'inclure toutes les fonctionnalités du mode DART-FT. La démarche n'est pas évidente car DART-Lux utilise une approche de modélisation très différente de celle de DART-FT.

DART simule tout type de paysages urbains ou naturels. Il peut simuler des couverts végétaux représentés par des objets 3D réalistes importés, des objets 3D schématiques créés en interne par DART ou des couverts représentés par un milieu turbide 3D. Dans cette thèse, les approches de modélisation et les implémentations de l'émission de SIF sont introduites et testées pour les deux modes de DART (*i.e.*, DART-FT et DART-Lux) et pour les deux méthodes de représentation de la végétation (facettes, turbide). L'introduction de la SIF dans DART a permis

d'évaluer l'impact de la structure 3D sur la SIF d'une forêt à feuilles caduques, en utilisant une scène forestière réaliste reconstruite à partir de données LiDAR. De plus, l'émission thermique et le bilan radiatif sont deux composantes importantes du bilan d'énergie qui quantifient l'échange d'énergie de la végétation par le rayonnement. Ils doivent être simulés avec précision avant de considérer l'échange d'énergie via des processus non-radiatifs. Dans cette thèse, nous introduisons également la modélisation de l'émission thermique et du bilan radiatif dans DART-Lux. L'objectif de ce travail est de fournir des éléments de base du transfert radiatif en vue du développement d'un modèle SIF 3D complet.

Cette thèse est organisée en cinq chapitres :

Le chapitre 1 est un chapitre introductif qui présente les concepts théoriques généraux sur la fluorescence, la fluorescence induite par le soleil et son utilisation pour le suivi du fonctionnement de la végétation avec la télédétection. Il présente également le modèle DART avec un accent particulier sur DART-Lux qui sera le plus considéré dans les chapitres suivants.

Le chapitre 2 présente la modélisation SIF dans DART-FT pour la végétation simulée comme des facettes et comme un milieu turbide 3D.

Le chapitre 3 présente la modélisation de la SIF dans DART-Lux pour la végétation simulée en tant que facettes et en tant que milieu turbide 3D. Une nouvelle méthode a été développée pour introduire l'émission SIF pour le traçage de chemin bidirectionnel. De plus, la végétation turbide a été introduite dans DART-Lux en incluant l'émission SIF.

Le chapitre 4 montre l'impact de la structure de la végétation sur l'émission et l'observation de la SIF. Il s'agit d'une étude théorique avec des scènes forestières reconstruites à partir du LiDAR.

Le chapitre 5 présente la modélisation de l'émission thermique et du bilan radiatif dans DART-Lux pour des éléments de scène simulés comme des facettes et comme des volumes (milieu turbide, fluides).



# Chapter 1

## **Context: Solar-Induced Fluorescence and DART model**

This thesis is centered on the modeling of chlorophyll solar-induced fluorescence in the DART model. In addition to the presentation of DART, this chapter introduces the context and associated questions: what is the chemical process behind the fluorescence emission and does it only happen for chlorophyll molecules? When was the fluorescence and particularly the chlorophyll fluorescence discovered? What about the correlation between chlorophyll fluorescence and photosynthesis? Why is it important to have models that simulate the SIF? What is the state of the art of fluorescence modeling?

### **1.1 Fluorescence**

Fluorescence is considered as a photoluminescence phenomenon among others like phosphorescence and delayed fluorescence. Photoluminescence is the type of luminescence (*i.e.*, emission of photons from electronically excited chemical species) of which the excitation is due to the absorption of light. The first reported observation of fluorescence was as early as 1565 when the Spanish medical practitioner Nicolás Monardes described the blue color of the water infusion of a type of wood known as *Lignum nephriticum* under certain conditions. The



# CHAPTER 1: CONTEXT: SOLAR-INDUCED FLUORESCENCE AND DART MODEL

term fluorescence was introduced by Stokes, (1852), from “fluorspar” analogously to “opalescence” which was also derived from the name of a mineral. He found that the emitted light has a longer wavelength than the absorbed light when he illuminated a solution of quinine sulfate with ultra-violet light and observed a blue light (Valeur, 2012b).

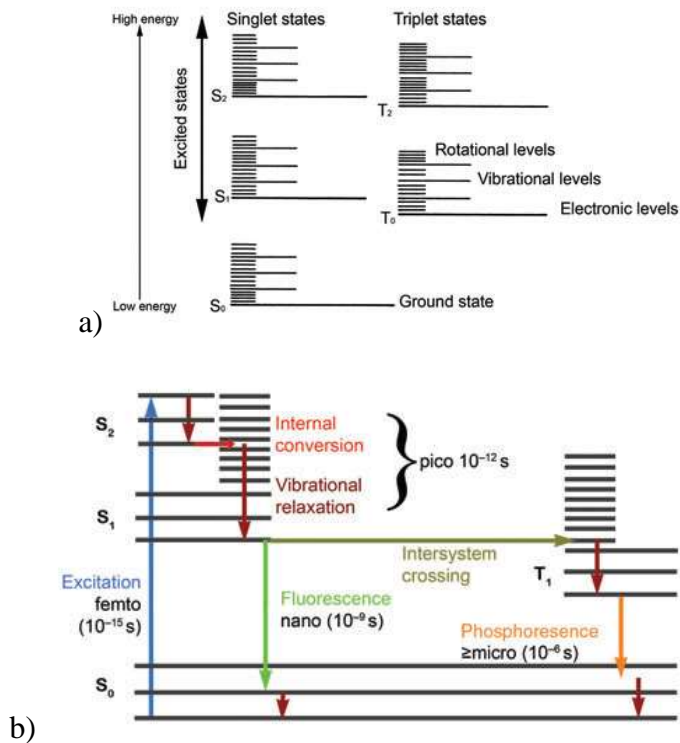


Figure 1-1: Jablonski diagram: a) Energy states, b) Possible transitions and their time lapses. (Lichtman & Conchello, 2005)

After absorbing a quantum of light, a fluorescent molecule passes to a vibrational level associated to a higher electronic state. The excited state is unstable and the molecule needs to dispose of its excess of energy. First, the excited molecule can lose energy through non-radiative (*i.e.*, without photon emission) state transitions (*e.g.*, internal conversion, vibrational relaxation) that occur in a time lapse in the order of  $10^{-12}$  s allowing the molecule to pass to the lowest vibrational level of an electronic state by transferring energy to other molecules and generating heat. Then, in a time lapse in the order of  $10^{-9}$  s, it can release the remaining energy by emitting a photon, and this emission is called fluorescence. Because the loss of energy due non-radiative state transitions is faster than fluorescence emission, the latter usually occurs at wavelengths larger than the incident light and therefore having less energy. This is called the

## 1.2 SOLAR-INDUCED CHLOROPHYLL FLUORESCENCE (SIF)

Stokes' Law. However, the emission can, with a low probability, be at a lower wavelength. This may seem to contradict the energy conservation principle, nevertheless, it happens because a small fraction of molecules have a vibrational level higher than 0 at normal temperature, and can emit a photon with higher energy than that of the absorbed photon (Valeur, 2012a). The electronic states and the transitions between them are usually illustrated with a Jablonski diagram (Jabłoński, 1935) as shown in Figure 1-1.

### 1.2 Solar-induced chlorophyll fluorescence (SIF)

The chlorophyll molecule has also shown to be fluorescent. The first reported observation of chlorophyll fluorescence induced by solar radiation was made by Brewster (1834) who noticed that the color of an alcoholic extract of chlorophyll hit by sunlight was a brilliant red. The photosynthetic process (photochemical quenching), the heat dissipation (non-photochemical quenching) and the fluorescence emission are three processes in competition over the absorbed energy by a chlorophyll molecule. Hence, the chlorophyll fluorescence emission is closely linked with photosynthetic activity. This link was first noticed by Müller (1874) and confirmed by Kautsky & Hirsch (1931) who noted the correlation between the variation of fluorescence emission and CO<sub>2</sub> assimilation. This correlation was further studied by McAlister & Myers (1940), Kautsky & Zedlitz (1941) and Kautsky et al. (1960). Since then, the fluorescence emission is considered as a proxy for photosynthetic activity (Baker, 2008).

### 1.3 Remote sensing of SIF

Being an electromagnetic radiation, the passive chlorophyll fluorescence of canopies induced by sunlight can be studied via remote sensing. Chlorophyll solar-induced fluorescence emission spectral range [640-850 nm] is spectrally overlapping with sunlight reflected by vegetation canopies. Moreover, because of its small quantum yield which is typically between 0.5 and 3% and usually does not exceed 10% in vivo (Porcar-Castell et al., 2014), it represents a small fraction of the light reflected by vegetation canopies (*e.g.*, 2-6% at 740 nm (Campbell et al., 2008)). Nevertheless, the retrieval of SIF is possible in absorption bands of the incident radiation, where the SIF has a larger relative contribution to the total signal from the canopy.

Some techniques use the atmospheric oxygen O<sub>2</sub>A and O<sub>2</sub>B absorption bands located inside the SIF spectrum around 760 nm and 687 nm respectively, to quantify the SIF observed in these bands (Fournier et al., 2012; Moya et al., 2004). Other techniques utilize the Fraunhofer lines of the solar spectrum to retrieve the SIF (Frankenberg et al., 2011; Guanter et al., 2012). The development of these techniques allowed accurate retrievals of SIF from in situ (Cogliati et al., 2015; Fournier et al., 2012), airborne (Rossini et al., 2015) and even spaceborne (Guanter et al., 2012) sensors. This enabled to use SIF remote sensing for monitoring the functional state of vegetation, by early stress detection (Ač et al., 2015), tracking photosynthetic activity and estimating the gross primary production (Campbell et al., 2019; Guanter et al., 2014; X. Liu et al., 2019; Z. Liu et al., 2019; P. Yang et al., 2021). This potential of SIF led the European Space Agency (ESA) to select a satellite dedicated for SIF observation Fluorescence Explorer (FLEX) as its 8<sup>th</sup> Earth Explorer mission (Drusch et al., 2017).

## **1.4 Modeling of SIF emission and observations**

Although SIF emission is highly correlated with instantaneous photosynthetic activity and gross primary production, it is also highly impacted by several other confounding factors. Indeed, it is directly linked with the PAR absorption, which depends on the sun direction, the atmospheric conditions and also the 3D architecture and optical properties of the canopy. Besides, the SIF emitted within the canopy interacts with all canopy elements and can undergo wavelength-dependent phenomena such as scattering and re-absorption by the different canopy elements or the soil. Therefore, only a small fraction of the emitted SIF can escape from the canopy into the upward hemisphere and is measured by remote sensing sensors. These interactions greatly depend on the canopy 3D architecture of the canopy and on the wavelength. In addition, the SIF signal above the canopy (*i.e.*, canopy SIF radiance) is anisotropic, which makes it more complex to extrapolate the SIF emission of the canopy from a single remote sensing observation. Therefore, for an accurate interpretation of SIF remote sensing observations, a comprehensive and deep understanding of three consecutive processes is essential. 1) Interception and absorption of photosynthetically active radiation by leaf pigments directly or after interacting with the atmosphere and all canopy elements. 2) Emission of SIF at photosystem level based on the absorbed PAR with a certain quantum efficiency that depends on photosynthetic and

## 1.4 MODELING OF SIF EMISSION AND OBSERVATIONS

heat dissipation efficiencies which in turn depend on local climatological conditions. 3) Propagation of SIF radiation through the canopies and its interaction with all canopy elements including leaves, soil, woody elements etc. until reaching the sensor.

Models that accurately simulate SIF emission and observations are essential tools for understanding and interpreting the SIF measurements, and extracting useful information from them. For this objective, models should consider each of the many parameters (*e.g.*, 3D architecture and optical properties of the canopy, illumination conditions, environmental parameters) that influence SIF emission. Second, models should accurately simulate the measured SIF signal as a function of the emitted SIF, the canopy properties and the observation configuration. Third, models should help in understanding the links between the within canopy SIF emission, the photosynthetic activity and the gross primary production of vegetation. Finally, models should allow performing sensitivity studies difficult or even impossible to do on real canopies. They should also allow the generation of synthetic databases or look-up tables that can be used by inversion algorithms to estimate SIF related parameters (*e.g.*, fluorescence quantum efficiency) and other vegetation functional state parameters (*e.g.*, CO<sub>2</sub> assimilation rate, gross primary production). In short, they should allow to link the SIF measurements to the real-time photosynthetic activity. Among these models, we can distinguish leaf-level SIF models that simulate radiative transfer within the leaf to provide leaf-level SIF emission, and canopy level models that upscale the leaf-level SIF models to the canopy level by simulating within-canopy radiative transfer.

### 1.4.1 Leaf-level modeling

Leaf-level SIF models include semi-empirical models such as FluorMODleaf (Pedrós et al., 2010) and Fluspect (Vilfan et al., 2016, 2018) that are based on the PROSPECT model (Jacquemoud & Baret, 1990). They simulate leaf hemispherical spectral optical properties and leaf SIF emission using the leaf biochemical properties and photosystem level fluorescence quantum efficiency as input parameters. Figure 1-2 shows an example of the output of the widely used leaf-level SIF model Fluspect. (Input parameters: chlorophyll content: 30  $\mu\text{g. cm}^{-2}$ , carotenoid content: 10  $\mu\text{g. cm}^{-2}$ , dry matter content: 0.01  $\text{g. cm}^{-2}$ , equivalent water thickness: 0.012  $\text{cm}$ , structure coefficient: 1.8, fluorescence yields: PSI: 0.002, PSII: 0.01). These are four excitation-emission fluorescence matrices. An element  $f_{i,j}$  of each matrix multiplied by the leaf irradiance  $E_i$  at the spectral band  $i$ , gives the emitted SIF exitance  $F_{i,j}$  at

the spectral band  $j$  induced by  $E_i$ . The leaf SIF exitance  $F_j$  emitted at spectral band  $j$  is the sum of the SIF exitance  $F_{i,j}$  due to all the  $N_{exc}$  excitation bands:

$$F_j = \sum_{i=1}^{N_{exc}} E_i \cdot f_{i,j} \quad (1.1)$$

The row vector of spectral SIF for the  $N_{em}$  emission bands  $(F_j)_{j \in \{1..N_{em}\}}$  can be written as the product of the row vector spectral irradiance  $(E_i)_{i \in \{1..N_{exc}\}}$  by the SIF excitation-emission matrix  $(f_{i,j})_{\substack{i \in \{1..N_{exc}\} \\ j \in \{1..N_{em}\}}}$  for the corresponding excitation and fluorescent bands. According to the Stokes' Law, if  $N_{exc} = N_{em}$ , these matrices should be upper triangular (*i.e.*,  $f_{i,j} = 0, \forall i > j$ ). However, they can have non-null very low values below the diagonal. This is not in contradiction with the energy conservation principle as explained in Section 1.1.

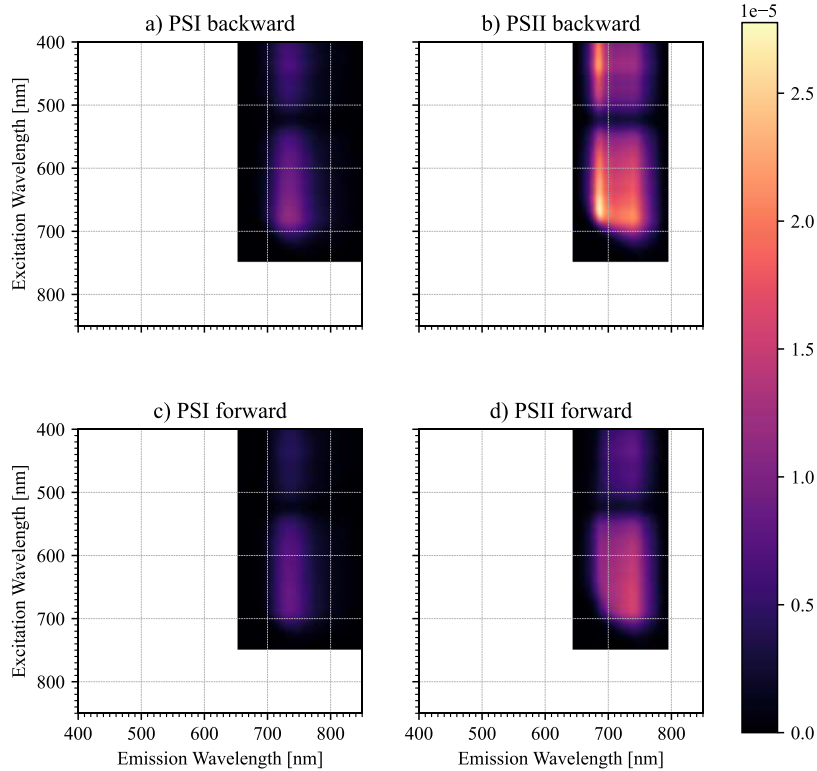


Figure 1-2: Image representations of four fluorescence excitation-emission matrices at 1 nm spectral resolution simulated by the Fluspect model. White pixels represent exact 0 values, black pixels represent positive values close to 0.

Leaf SIF models also include 3D radiative transfer models that use accurate (Kallel, 2020b) or less accurate (Sušila & Nauš, 2007) 3D descriptions of the leaf to simulate within leaf radiative

## 1.4 MODELING OF SIF EMISSION AND OBSERVATIONS

transfer and to compute leaf spectral reflectance, transmittance and fluorescence. Leaf SIF models are usually combined with canopy radiative transfer models to upscale the SIF emission from leaf to canopy level.

### 1.4.2 Canopy level modeling

Ideally, a canopy-level SIF model should simulate accurately all the radiative and non-radiative processes that impact the SIF signal. Considering the accurate 3D architecture of vegetation canopies, it should simulate the propagation of sunlight to quantify the absorbed PAR, and the propagation of SIF radiation to estimate the measured signal. Moreover, it needs to compute the leaf-level SIF emission based on the absorbed PAR, possibly using a leaf-level SIF model, and considering the local parameters that influence SIF emission (*e.g.*, leaf temperature). To this end, the full energy balance needs to be modeled with its radiative (*i.e.*, full radiative budget from visible to thermal infrared domain), and non-radiative (*e.g.*, photosynthesis, turbulence, heat exchanges) components. The existing SIF models that simulate the full energy balance are 1D only. They make a very limiting assumption of horizontally homogenous canopies, neglecting the actual 3D structure of vegetation canopies. They represent the canopy by homogeneous turbid layers characterized by a Leaf Area Index (LAI) and a Leaf Angular Distribution (LAD). This is the case of the SCOPE model (van der Tol et al., 2009) and its multi-layered version mSCOPE (P. Yang et al., 2017). They use the Fluspect model to simulate dark-adapted leaf fluorescence, and then weight the SIF emission by multiplicative factors derived from a 1D energy balance algorithm in order to consider the effect of local climatology on SIF emission. These models are, to some extent, adapted for homogeneous and closed crop canopies, but they are much less adapted for forest heterogeneous covers and crop canopies with a clear row distribution that can provoke important effects related to 3D structure both for radiation absorption and remote sensing observations. They also neglect some canopy elements such as woody elements and local topography. In recent years, several 3D canopy SIF models have been developed. They usually result from already existing 3D radiative transfer models combined with a leaf-level SIF model. For instance, FluorFLIGHT (Hernández-Clemente et al., 2017) is based on the FLIGHT model (North, 1996), FLiES-SIF (Sakai et al., 2020) and FluorFLiES (Gao et al., 2022) are based on the FLiES (Kobayashi & Iwabuchi, 2008) model, the FluLCVRT (Kallel, 2020b) is based on the LCVRT model (Kallel, 2020a) and FluorWPS (Zhao et al., 2016) is based on the WPS model (Zhao et al., 2015). However, none of these

models simulate the full 3D energy balance. Hence, they cannot compute the multiplicative factors to get the steady state leaf SIF from the dark-adapted leaf SIF based on the local climatology. It is left up to the user to input directly the steady state fluorescence quantum efficiency, which is challenging to measure for all the leaves. This is also the case for the DART model. However, the latter offers the possibility to import fluorescence multiplicative factors computed by other models (*e.g.*, the  $\eta$  factors computed by SCOPE) to weight the leaf SIF emission according to the local climatology. Obviously, importing information from a 1D model (SCOPE) to a 3D model (DART) is only an approximation. For example, the  $\eta$  factor can have a large horizontal variation depending on the local conditions of each individual leaf.

## 1.5 DART model

DART (Discrete Anisotropic Radiative Transfer) is one of the most comprehensive 3D radiative transfer models in optical remote sensing domain. It is developed in CESBIO (Centre d'Etudes Spatiales de la Biosphère) since 1992. It simulates the 3D radiative budget and remote sensing observations from ultraviolet to thermal infrared of any natural or urban 3D landscape for any experimental configuration (*e.g.*, sun direction, atmosphere, etc.) and instrumental configuration (*e.g.*, viewing direction, spatial resolution, etc.) for spaceborne, airborne and in situ imaging spectro-radiometers (scanners, cameras, etc.) and LiDAR (Light Detection And Ranging). To this end, DART has four main modules: 1) “Directions” is used for subdividing the  $4\pi$  space into a finite number  $N$  of discrete directions  $\Omega_n$  having solid angles  $\Delta\Omega_n$  and  $P$  ( $P \leq N$ ) angular sectors. 2) “Phase” is used for computing the optical properties, temperature properties and phase functions for the user defined surfaces and volumes, and for the specified spectral bands. 3) “Maket” is used to create the mock-up from the user-defined scene elements. A Python toolbox, called “DAO” is also provided with DART to allow the automatic creation of mock-ups directly from external data such as 3D LAI information derived from LiDAR data. It can replace the “Maket” module that is in general used with the graphical user interface. 4) “Dart” is the module that simulates radiative transfer in the scene using geometric and optical information generated by the three previous modules in order to generate the user-selected radiative products (*e.g.*, 3D radiative budget and / or remote sensing signal). Each DART spectral band can have any of three radiation modes: 1) R mode: the sun is the only source of

radiation. 2) T mode: thermal emission of scene elements and the atmosphere is the only source of radiation. 3) R + T mode: both the solar radiation and thermal emission are considered. Moreover, three modes (i.e., DART-FT, DART-RC and DART-Lux) are used to simulate radiative transfer in the 3D scenes. These modes are presented in the next sub-sections.

### 1.5.1 DART-FT

DART-FT is the standard mode of DART. It is called FT, as Flux Tracking, because it tracks radiation using an adaptation of the discrete ordinates method in a finite number  $N$  of discrete directions ( $\Omega_n, \Delta\Omega_n$ ) over the  $4\pi$  space (Yin et al., 2013) in a scene made of voxels (Figure 1-3). This approach is iterative: radiation intercepted at iteration  $i$  is scattered at iteration  $i + 1$ . Using the pure discrete ordinates method, each ray intercepted at a given iteration would give rise to  $N$  scattered rays at the following iteration, which would result in an exponential growth of the number of tracked rays, and therefore a huge and unmanageable number of rays. To avoid this exponential growth, pragmatic approximation approaches such as the use of barycenters of scattering points on surfaces and in voxels are used, which greatly reduces the number of scattering points, and consequently the number of scattered rays. The DART-FT mode has two major limitations. 1) It is not efficient in terms of computation time and memory usage for image simulation. It spends computation resources to track and to store every single ray even if this ray has not a real contribution to the signal of interest. 2) The discretization of the  $4\pi$  space into a finite number of discrete directions and the inevitable use of approximations to limit the number of rays is a source of inaccuracies and discretization artefacts. On the other hand, since all the radiation is tracked inside the scene, it is possible to know the amount of radiation that is intercepted, scattered or absorbed everywhere in the scene. Therefore, DART-FT is efficient for simulating the radiation budget of canopies. Moreover, because of its iterative approach, a single simulation can provide products at different scattering orders. In addition, an iterative process extrapolates the last iteration orders to the infinite scattering order.

The initial version of DART was only adapted to 3D vegetation canopies made of voxels either empty or filled with turbid medium, and to radiation in the shortwaves (Gastellu-Etchegorry et al., 1996). Other modelling processes were introduced later: use of facets to simulate surface elements in the voxelized scene (Gastellu-Etchegorry et al., 2004), radiative transfer in the atmosphere (Gascon et al., 2001), thermal emission for simulating the remote sensing signal



and radiative budget in the thermal infrared domain (Guillevic et al., 2003), and solar induced fluorescence (Gastellu-Etchegorry et al., 2017).

### 1.5.2 DART-RC

DART-RC is the DART radiative transfer mode for simulating the LiDAR signal of 3D scenes (Gastellu-Etchegorry et al., 2015) simulated by an array of voxels. It tracks radiation using a combination of the discrete ordinates method and forward Monte Carlo ray tracing. Its products include several types of LiDAR products (*e.g.*, waveforms, point clouds, photon counting).

### 1.5.3 DART-Lux

Since 2018, DART includes a new mode called DART-Lux (Wang et al., 2022). It is a bi-directional Monte Carlo radiative transfer method based on the open-source rendering engine LuxCoreRender (<https://luxcorerender.org>). DART-Lux uses Monte Carlo integration techniques to solve the Light Transport Equation. Monte Carlo integration is an integration method that allows to estimate the integral of a given function using only random sampling of points in the definition domain of this function and the evaluation of the function in these points.

The naïve Monte Carlo estimator for the integral  $I = \int_a^b f(x) \cdot dx$  of the 1D function  $f$  is:

$$\hat{I} = \frac{b-a}{N} \sum_{i=1}^N f(x_i) \quad (1.2)$$

with  $\{x_1, \dots, x_N\}$  are points uniformly sampled over the interval  $[a, b]$ .

This estimator is not biased: its expected value is the real value  $I$  of the integral (cf. Appendix 1-1). Therefore, it converges towards the real value when the number of samples is large enough.

The sampling of  $x_i$  can be done using any probability distribution function (PDF)  $p(x)$ , apart from the uniform distribution. In this case, the Monte Carlo estimator becomes:

$$\hat{I}_p = \frac{1}{N} \sum_{i=1}^N \frac{f(x_i)}{p(x_i)} \quad (1.3)$$

Ideally, the PDF should be chosen such that it has a similar shape to  $f$ . This technique is called “Importance Sampling” and is used to reduce the variance of Monte Carlo estimators.

The Monte Carlo integration method can easily be extended to estimate integrals over high dimensional integration domains. Its algorithmic complexity does not change with the dimension of the domains as it only depends on the number of sampled points. Therefore, it can be used to compute the radiance measurement  $L^{(j)}$  of pixel  $j$  of a simulated image given by the integral form of the Light Transport Equation:

$$L^{(j)} = \int_{\mathcal{D}} C^{(j)}(\bar{p}) \cdot dA(\bar{p}) \quad (1.4)$$

- $\bar{p}$ : light transport path.  $\bar{p}_k = (p_0, \dots, p_k)$  is a path of length  $k$  (*i.e.*,  $k$  segments and  $k+1$  vertices  $p_i$  with  $i \in [0, k]$ ).
- $\mathcal{D}$ : set of all possible light paths.  $\mathcal{D} = \bigcup_{k=1}^{\infty} \mathcal{D}_k$ , with  $\mathcal{D}_k$  the set of all paths  $\bar{p}_k$  of length  $k$ .
- $dA(\bar{p})$ : area product for path  $\bar{p}$ ; *e.g.*,  $dA(\bar{p}_k) = dA(p_0) \dots dA(p_k)$  with area  $dA(p_i)$  at vertex  $i$ .
- $C^{(j)}(\bar{p})$ : contribution function of path  $\bar{p}$  to the measurement  $L^{(j)}$  of pixel  $j$ .

When sampling random light paths for the Monte Carlo estimator of pixel radiance using the importance sampling technique, paths with higher contribution to the pixel radiance have higher chances to be sampled. The light path sampling starts from the light source (*i.e.*, forward direction) and from the sensor (*i.e.*, backward direction). Forward tracing is more efficient for sampling light sources with narrow solid angle of illumination and backward tracing for sensors with narrow fields of view (FOV) (Disney et al., 2000). The bi-directional tracing combines the forward and backward tracing and allows to benefit from the advantages of the two methods. Unlike the discrete ordinates method that spends computational resources to track all radiation over the scene even if it has a negligible impact on the simulated observation, the bi-directional path tracing (BDPT) algorithm, by sampling with higher probability light paths that have higher contribution to the image, it allows to preferentially track rays that contribute most to the required observations which makes it more computationally efficient for images simulation. Moreover, because its algorithmic complexity does not depend on the scene complexity, it is more and more efficient for large and complex scenes. DART-Lux takes advantage of the development of rendering algorithms in computer graphics. The BDPT algorithm implementation of the physical renderer LuxCoreRender has been selected and adapted to the remote sensing field, in the comprehensive and user-friendly framework of DART. The initial goal of the DART team was to introduce most of the functionalities of DART-FT and DART-RC into DART-Lux, with improved accuracy and lower computer and memory requirements, within the framework of DART and with the ability to switch seamlessly

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between modes. To this end, many physical and technical improvements and adaptations had to be made. Ten major modelling developments are listed here. 1) To overcome the hard coded 3-channel RGB limit in LuxCoreRender for simulations with any number of spectral bands. 2) To simulate radiance and reflectance remote sensing images (Wang et al., 2022; Wang & Gastellu-Etchegorry, 2021). 3) To support input and output formats of the DART framework. (DAO, SQL databases, images, etc.). 4) To implement radiative transfer modelling in the atmosphere in order to simulate BOA and TOA images. 5) To simulate LiDAR signal (X. Yang et al., 2022). 6) To simulate polarization mechanisms. 7) To implement the modeling of radiative transfer in scenes made of volumes filled with turbid medium and fluids. 8) To model solar-induced fluorescence. 9) To model thermal emission by the scene elements and the atmosphere. 10) To model the 3D radiative budget of 3D scenes.

Compared to DART-FT, DART-Lux greatly reduces computation time and memory needs for image simulation of large and complex scenes. It also usually improves accuracy and avoids artefacts due to discretization as it eliminates processes such as discretizing the  $4\pi$  space, voxelizing the 3D scene (Figure 1-3) and combining rays to reduce their number.

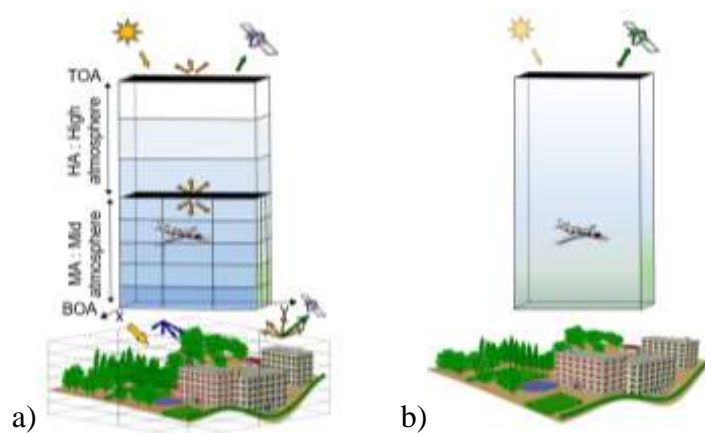


Figure 1-3: a) DART-FT voxelized scene b) DART-Lux scene: voxels are no more needed

### 1.6 Conclusion

This chapter presented historical and theoretical aspects about the fluorescence, and in particular chlorophyll solar-induced fluorescence and its great potential for monitoring real-time vegetation functioning status. It also presented the DART model, and in particular the DART-Lux mode and its BDPT algorithm which will be of interest in the next chapters.

## Appendix 1-1: Expected values of $\hat{I}$ and $\hat{I}_p$

$$\begin{aligned}
 E[\hat{I}] &= \frac{b-a}{N} \sum_{i=1}^N E[f(x_i)] \\
 &= \frac{b-a}{N} \sum_{i=1}^N \frac{1}{b-a} \int_a^b f(x) \cdot dx \\
 &= \int_a^b f(x) \cdot dx = I
 \end{aligned}$$

$$\begin{aligned}
 E[\hat{I}_p] &= \frac{1}{N} \sum_{i=1}^N E \left[ \frac{f(x_i)}{p(x_i)} \right] \\
 &= \frac{1}{N} \sum_{i=1}^N \int_a^b \frac{f(x)}{p(x)} \cdot p(x) dx \\
 &= \int_a^b f(x) \cdot dx = I
 \end{aligned}$$

## Appendix 1-2: Nomenclature

Symbol	Description	Unit
$E_i$	Irradiance at the spectral band $i$	$W \cdot m^{-2} \cdot \mu m^{-1}$
$F_j$	SIF exitance at the spectral band $j$	$W \cdot m^{-2} \cdot \mu m^{-1}$
$f_{i,j}$	Fluorescence matrix element for excitation band $i$ and emission band $j$	-
$F_{i,j}$	SIF exitance at the spectral band $j$ due to the excitation at the spectral band $i$	$W \cdot m^{-2} \cdot \mu m^{-1}$

$\hat{I}$	Monte Carlo estimator of the integral $I$ using the uniform probability density function.	-
$\hat{I}_p$	Monte Carlo estimator of the integral $I$ using the probability density function $p$ .	-
$L^{(j)}$	Radiance measurement of pixel $j$	$W.m^{-2}.\mu m^{-1}.sr^{-1}$
$N_{em}$	Number of emission bands	-
$N_{exc}$	Number of excitation bands	-

# Chapter 2

## **SIF modeling in DART-FT**

DART-FT is the initial DART mode that simulates radiative transfer based on the discrete ordinates method. It has two possible representations of vegetation: facets-based 3D objects representation and 3D voxelized turbid representation. In this chapter, the two approaches used for modeling the SIF emission and radiation propagation in DART-FT for the facets and turbid representations are presented. The first section is dedicated to the facets-based SIF simulation. It was the subject of a publication included in this thesis in which I am the second author. My main contribution was to design and prepare DART and SCOPE/mSCOPE simulations for comparing their simulations of the SIF signal, using the 1D models as reference models, as are generally accepted in the community. The second section presents SIF modeling in vegetation simulated as turbid medium. I participated in the design of this new modelling and implemented it in DART.

### **2.1 Vegetation simulated as facets**

#### **2.1.1 Modeling approach**

The implementation of SIF emission in DART-FT for vegetation simulated as facets consisted in imbedding the leaf-level SIF model Fluspect into DART-FT. Fluspect gives SIF excitation-emission matrices at 1 nm spectral resolution that are resampled to the user-specified spectral

bands of the DART simulation. It is important to note that the excitation spectral bands should cover all the excitation spectral interval (*i.e.*, [400 – 750 nm]) otherwise the SIF will be underestimated, and should not overlap otherwise the SIF will be overestimated. To include the SIF radiation, radiation fluxes vectors have 3 components: total flux components, and two SIF components for the photosystems PSI and PSII, respectively. Radiation fluxes with these 3 components are mechanistically tracked in the forward direction within the scene. Intercepted by a non-fluorescent or a fluorescent surface, the total, PSI and PSII radiation flux components are scattered or absorbed in the same way as the total flux. If the interacting surface is fluorescent, SIF radiation is added to the scattered PSI and PSII radiation components. This added SIF radiation is simulated by multiplying the total leaf irradiance by the relevant SIF excitation-emission matrix (PSI or PSII, backward or forward). The article of Malenovský et al. (2021) in Section 2.1.3 gives further details about SIF modeling in DART-FT for vegetation simulated as facets.

### 2.1.2 Results

Ideally, a radiative transfer model should be compared to real field measurements to assess its consistency. However, this comparison is very challenging in general, especially for 3D models. In order to be consistent with the very tiny and anisotropic SIF signal, a relevant comparison of a 3D SIF radiative transfer model with field measurement requires: 1) accurate 3D scene reconstruction that accounts for the field geometry and the plants 3D architecture, 2) bottom of atmosphere spectral irradiance with a good spectral resolution (*i.e.*,  $\leq 1$  nm), or accurate atmosphere parameters to simulate radiative transfer in the atmosphere, 3) steady-state fluorescence quantum efficiency at photosystems level or dark-adapted fluorescence quantum efficiency along with  $\eta$  multiplicative factors computed by a 3D energy balance model, 4) scene elements optical properties including leaves optical properties (*i.e.*, spectral reflectance and transmittance) that need to be inverted to retrieve the Fluspect input parameters to compute the leaf level fluorescence matrices. Most of these input parameters are not straightforward to obtain and require long processes. For instance, the fluorescence quantum efficiency, a major key parameter that drives SIF emission, is highly variable in time and space and is challenging to measure. Hence, although several SIF measurements are available at different levels (in-situ, airborne, satellite), a complete dataset ready to use for comparison with 3D radiative transfer models was not available. Therefore, in order to assess the accuracy of DART-FT SIF modeling,

## 2.1 VEGETATION SIMULATED AS FACETS

we performed a model-to-model comparison with a model that is considered as a reference SIF model in the community. The agreement of two models that use completely different approaches can be a first assessment of the models' consistency provided that they are tested in exactly the same conditions. Unfortunately, the only reference model is 1D only. This approach does not replace the need of comparisons with real field SIF measurements. Bearing this in mind, we have compared the SIF modeling in DART-FT with SCOPE (van der Tol et al., 2009) and its multi-layered version mSCOPE (P. Yang et al., 2017). They are 1D models and are considered as a “reference” for SIF modeling. They represent vegetation as homogeneous turbid layers, with a possible vertical heterogeneity in mSCOPE. Turbid medium is a statistical representation of vegetation using a leaf area volumetric density  $u_l$  ( $m^2 \cdot m^{-3}$ ) and a Leaf Angular Distribution (LAD)  $\frac{g(\theta_l)}{2\pi}$ . It is equivalent to an infinite number of infinitely small plane elements distributed according to  $\frac{g(\theta_l)}{2\pi}$  and having a total area per volume unit equal to  $u_l$ . To approximate this representation, the equivalent DART mock-up is constructed as a “quasi-turbid” medium: a cloud of very small facets distributed according to the same LAD  $\frac{g(\theta_l)}{2\pi}$  and having a total area per volume unit equal to  $u_l$ . The comparison of DART-FT simulation for quasi-turbid medium with SCOPE and mSCOPE showed a good agreement between the models, as presented in the article of Malenovský et al., (2021). (cf. Section 2.1.3)

### 2.1.3 Article:





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## Discrete anisotropic radiative transfer modelling of solar-induced chlorophyll fluorescence: Structural impacts in geometrically explicit vegetation canopies

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## ABSTRACT

Solar-induced fluorescence (SIF) is a subtle but informative optical signal of vegetation photosynthesis. Remotely sensed SIF integrates environmental, physiological and structural changes that alter photosynthesis at leaf, plant and canopy scales. Radiative transfer models are ideally suited to investigate the complex sources of variability in the SIF signal to enable the interpretation of SIF retrievals from airborne and space-borne platforms. Here, we coupled the FluSpec-Cx model of leaf optical properties and chlorophyll-*a* fluorescence with the Discrete Anisotropic Radiative Transfer (DART) model to upscale SIF from individual leaves to three-dimensional (3D) structurally explicit canopies. For two-dimensional homogeneous (turbid-like) canopies, DART-SIF was nearly identical to SIF simulated in two existing models, SCOPE and mSCOPE (RMSE < 0.221 W.m<sup>-2</sup>.μm<sup>-1</sup>.sr<sup>-1</sup>). DART simulations in geometrically explicit 3D canopies offered four important insights regarding the influence of vegetation structure on the multi-angular top-of-canopy SIF signal. First, changes in the 3D canopy architecture of maize crops, represented by leaf density (leaf area index), and plant clumping (canopy closure) had a larger impact on SIF than the modelled photosynthetic efficiency distinction between sun-adapted and shade-adapted foliage. Second, clumping of leaves at the crop and stand levels was identified as one of the key driving factors of multi-angular anisotropy of red and far-red SIF (686 and 740 nm) for both maize and eucalyptus canopies. Third, non-photosynthetic woody material had a significant impact on top-of-canopy SIF in modelled 3D forest stands. Wood shadowing decreased the photosynthetically active radiation absorbed by green leaves, and consequently the SIF emissions, by 10% in sparse and 17% in dense eucalyptus stands. The wood obstruction (blocking) effect, quantified as a relative difference of SIF escape probabilities from canopies with and without wood in the nadir viewing direction, decreased far-red SIF by 4–6% but it had a smaller and sometimes positive influence (by less than 2%) on red SIF. Fourth, DART 3D radiative budget profiles revealed that the majority of the SIF signal from a dense eucalyptus stand originated from the top 25% of the simulated canopy. Interestingly, the introduction of bark-covered woody elements did not alter the simulated balance and omnidirectional escape factor of red SIF in this upper canopy part but did raise significantly both of them in case of far-red SIF. These results demonstrate the importance of 3D radiative transfer and radiative budget simulations for investigating SIF interactions in structurally complex plant canopies and for a better understanding of spatiotemporal and multi-angular remote sensing SIF observations.

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### 1 **1. Introduction**

2       The potential for airborne and spaceborne monitoring of plant productivity has motivated  
3 optical remote sensing (RS) scientists since the launch of first Earth observing satellites (Ashley  
4 and Rea 1975; Blair and Baumgardner 1977). The faint signal of chlorophyll *a* fluorescence  
5 has been the target of vegetation RS for several decades (Rosema et al. 1991). Although recent  
6 technological advances in narrow-band imaging spectroscopy provide the first estimates of  
7 solar-induced chlorophyll fluorescence (SIF) from space (Frankenberg et al. 2011; Guanter et  
8 al. 2007; Joiner et al. 2011), the retrieval and use of the subtle SIF signal emitted in the red and  
9 near-infrared spectral regions to assess plant productivity is fraught with natural complexity of  
10 vegetated landscapes. Hence, RS applications of SIF, including physiological principles,  
11 instruments, measurement techniques and computer models (Mohammed et al. 2019), need a  
12 further development to improve our understanding and correct interpretation of the diurnal,  
13 seasonal, and interannual variabilities in the SIF signal observed with RS instruments at local,  
14 regional and global spatial scales. In particular, SIF variability originating from multiple  
15 scattering and reabsorption within structurally complex vegetation canopies is poorly  
16 understood, as are optical interactions in topographically rough and spatially heterogeneous  
17 natural and man-made landscapes (Zhang et al. 2020).

18       Radiative transfer modelling is a well-established and inseparable part of modern optical  
19 RS methods (Myneni and Ross 2012). Computer simulated radiative transfer in vegetation  
20 (Widlowski et al. 2015) has been used for local and global sensitivity analyses of various RS  
21 phenomena (e.g., Malenovský et al. 2008; Verrelst and Rivera 2017; Verrelst et al. 2010), and  
22 also for retrieval and interpretation of quantitative vegetation descriptors from remotely sensed  
23 spectral observations obtained through various inversion procedures (e.g., Croft et al. 2020;  
24 Malenovský et al. 2013; Verrelst et al. 2019). One of the most frequently used and well-  
25 established leaf-scale RTMs is PROSPECT (Féret et al. 2020; Féret et al. 2017; Jacquemoud  
26 and Baret 1990; Malenovský et al. 2006). Its first clone designed to simulate the chlorophyll-*a*  
27 fluorescence emission in plant leaves was FluorMODleaf (Pedrós et al. 2010), followed by  
28 computationally simpler Fluspect-B (Vilfan et al. 2016) and Fluspect-Cx (Vilfan et al. 2018).  
29 The Fluspect models reproduce leaf optical properties between 400 and 2500 nm together with  
30 3D matrices of forward- and backward-emitted SIF per wavelength of photosynthetically active  
31 radiation (PAR) incident on the adaxial side of a dark-adapted leaf. Besides these semi-  
32 empirical models, physical 3D leaf fluorescence RTMs have been developed, e.g., the Monte

33 Carlo (MC) Photon Transport (Sušila and Nauš 2007) or the Fluorescence Leaf Canopy Vector  
34 Radiative Transfer model (Kallel 2020). The MC models are, however, computationally  
35 demanding and, therefore, less suitable for an operational use in routine applications.

36 Models of SIF radiative transfer are developed hand-in-hand with the RS experimental  
37 work conducted at leaf as well as canopy scales (Aasen et al. 2019). Leaf RTMs are usually  
38 embedded in canopy-scale RTMs that can be classified according to the canopy representation  
39 as one-dimensional (1D) or three-dimensional (3D). Strengths and weaknesses of available  
40 canopy RTM types are reviewed in Malenovský et al. (2019). 1D models, such as SAIL  
41 (Verhoef 1984), were designed for a horizontally homogeneous canopy with structural, optical  
42 and biochemical variability only in the vertical dimension (e.g., mono-species crops). The most  
43 frequently used SIF model for 1D canopies is a SAIL's successor called SCOPE (van der Tol  
44 et al. 2009; van der Tol et al. 2019; Yang et al. 2020a), recently extended for multi-layered  
45 canopies as mSCOPE (Yang et al. 2017). Both SCOPE models are not modelling just radiance  
46 and SIF transfer but also soil-vegetation-atmosphere temperature and energy balances,  
47 including photosynthetic processes. SCOPE is frequently used for its simplicity and robustness,  
48 but its 1D architecture is unsuitable for complex multi-species ecosystems with structurally  
49 heterogeneous canopy layers and rough topography (e.g., boreal forests or savannas; Liu et al.  
50 2019a). Therefore, several 3D RTMs have been equipped with the ability to scale SIF from  
51 leaves to canopies to better capture the influence of structural heterogeneity of vegetation  
52 canopies. FluorWPS is a 3D MC ray-tracing SIF model (Zhao et al. 2016) that was developed  
53 and tested on 3D agricultural crops (Tong et al. 2021). Flux tracking of SIF simulated in the  
54 Discrete Anisotropic Radiative Transfer (DART) model (Gastellu-Etchegorry et al. 1996) was  
55 used to assess its multi-angular anisotropy in 3D maize canopies (Gastellu-Etchegorry et al.  
56 2017). The FluorFLIGHT 3D model, developed from FLIGHT (North 1996), supported  
57 assessment of Mediterranean oak forest water stress and *Phytophthora* infections from airborne  
58 SIF data (Hernández-Clemente et al. 2017). Finally, the FLiES MC model (Sakai et al. 2020)  
59 was used to interpret space-borne SIF of Amazonian forests (Köhler et al. 2018).

60 Despite the fact that all RTMs rely on simplifications and assumptions, they are powerful  
61 tools to investigate the optical interactions of SIF, which is needed for scaling and interpretation  
62 of the SIF signals acquired by proximal, airborne and spaceborne instruments (Bendig et al.  
63 2020; Gamon et al. 2019; Wyber et al. 2017). The main goal of this paper is to demonstrate the  
64 ability of the DART model coupled with Fluspect-Cx to assess the influence of canopy 3D

## 2.1 VEGETATION SIMULATED AS FACETS

65 architecture on the top-of-canopy SIF ( $SIF_{TOC}$ ) for cropland and forested environments that are  
66 difficult or even infeasible to investigate directly. DART simulations in this study address three  
67 primary research questions. First, in absence of a suitable 3D validation measurements and to  
68 verify their modelling consistency, do the DART, SCOPE and mSCOPE models provide  
69 comparable estimates of  $SIF_{TOC}$  for structurally homogenous vegetation in form of a turbid  
70 medium? Second, what is the  $SIF_{TOC}$  impact originating from biochemical leaf fluorescence  
71 efficiencies ( $f_{qe}$ ), varying for sun- and shade-adapted leaves, in comparison to increasing leaf  
72 density and clumping of maize (*Zea mays L.*) canopies? And third, what are the effects of woody  
73 trunks and branches on simulated  $SIF_{TOC}$ , SIF fluxes and escape factors from 3D forest  
74 abstractions of dense and sparse Australian white peppermint (*Eucalyptus pulchella*) stands?

## 75 2. Material and Methods

### 76 2.1 Implementation of leaf chlorophyll fluorescence in DART

77 We used the 3D DART model as the pilot RTM of this study. DART, being developed by  
78 researchers from the CESBIO Laboratory in Toulouse for more than 20 years (Gastellu-  
79 Etchegorry et al. 1996), was successfully cross compared with other state-of-the-art RTMs  
80 within the RAMI exercise (Widlowski et al. 2015). It produces at-sensor top-of-atmosphere  
81 (TOA) and bottom-of-atmosphere (BOA) multi-angular RS images by tracking optical and  
82 thermal photon fluxes through any type of 3D landscape with atmosphere (Gastellu-Etchegorry  
83 et al. 2015). Additionally, it calculates the quantitative 3D radiative budget, i.e., fluxes of  
84 intercepted, absorbed, reflected and emitted radiation, in the optical spectral domain (400-2500  
85 nm) (Gastellu-Etchegorry et al. 2004). The presence of woody material was implemented in  
86 DART in 2008 (Malenovský et al. 2008), and radiative transfer of Fluspect-Cx modelled SIF  
87 emissions in 2017 (Gastellu-Etchegorry et al. 2017). The Fluspect-Cx implementation followed  
88 the approach that was previously applied to couple DART with the PROSPECT-D model (Féret  
89 et al. 2017), taking advantage of both models' computational similarities and commonalities in  
90 input/output handling. The DART version 5.7.3, used in this work, simulates SIF radiative  
91 transfer and budget for 3D vegetation canopies constructed from geometrically explicit  
92 triangular objects (facets). Based on user-defined input parameters (i.e., leaf chlorophyll  $a+b$ ,  
93 total carotenoid and brown pigment contents, equivalent water thickness, dry leaf mass per area,  
94 leaf mesophyll structural parameter and specific fluorescence efficiencies), Fluspect generates  
95 four SIF matrices ( $M_{xyij}$ ), where  $x$  is the photosystem PSI or PSII,  $y$  is the backward or forward

96 direction relative to radiation incident direction,  $i$  is the 1 nm excitation band in the  
 97 photosynthetically active spectral region from 400 to 750 nm ( $i \in [1 \text{ I}]$ ), and  $j$  is the 1 nm emitted  
 98 SIF band ( $j \in [1 \text{ J}]$ ) in the spectral region from 640 to 850 nm. Consequently, the Fluspect SIF  
 99 leaf exitance ( $F_{xyj}$ ) at band  $j$  (1 nm bandwidth) due to irradiance ( $E_i$ ) in band  $i$  is:

$$100 \quad F_{xyj} = M_{xyij} \cdot E_i. \quad (1)$$

101 In contrast to Fluspect, DART works with any number of spectral bands that can have any  
 102 bandwidth, for example with U excitation bands  $\lambda_u$  and V fluorescence bands  $\lambda_v$ . Hence, in  
 103 DART, a leaf irradiance ( $E_u$ ) leads to the leaf exitance:

$$104 \quad F_{xyv} = M_{xyuv} \cdot E_u, \quad (2)$$

105 where  $M_{xyuv}$  is derived from the Fluspect matrices ( $M_{xyij}$ ) using an interpolation on spectral  
 106 bands ( $\Delta\lambda_u = \sum \alpha_{ui} \cdot \Delta\lambda_i$ ,  $\Delta\lambda_v = \sum \beta_{uj} \cdot \Delta\lambda_j$ ) and the two-step weighted arithmetic averaging:

$$107 \quad M_{xyuv} = \frac{\sum_j \beta_{uj} \cdot \Delta\lambda_j \cdot M_{xyuj}}{\sum_j \beta_{uj} \cdot \Delta\lambda_j}, \text{ where} \quad (3)$$

$$108 \quad M_{xyuj} = \frac{\sum_i \alpha_{ui} \cdot \Delta\lambda_i \cdot M_{xyij}}{\sum_i \alpha_{ui} \cdot \Delta\lambda_i}. \quad (4)$$

109 DART spectral leaf SIF exitance is accurate only if the  $u$  bands cover the entire SIF excitation  
 110 spectral interval and if they do not overlap. Similarly, it simulates the whole SIF domain only  
 111 if the  $v$  bands cover the whole SIF emission spectral interval.

112 The Fluspect calibration optical parameters (i.e., specific absorption coefficients, refractive  
 113 index of mesophyll cell walls and water, etc.) are stored in an external table called Optipar. We  
 114 used the Optipar table released in 2015. Additionally to the standard PROSPECT leaf  
 115 biochemical and structural inputs, Fluspect requires leaf fluorescence quantum efficiencies  
 116 ( $fqe$ ), in DART referred to as fluorescence yields, for PSI and PSII. The specification of  $fqe$   
 117 values in DART is flexible. They can be entered per individual foliage facet or specified as  
 118 general parameters that represent all leaves or a group of leaves in a given canopy. Biologically  
 119 meaningful foliage groups are, for instance, sunlit (i.e., leaves exposed to direct sun radiation)  
 120 and shaded leaves (i.e., leaves in the shadow of other phytoelements), or sun-adapted (i.e.,  
 121 leaves exposed most of the time to a direct sun radiation and subsequently adapting their  
 122 pigment pools for a high photoprotective capacity) and shade-adapted leaves (i.e., leaves  
 123 growing most of their lifespan under a low-intensity diffuse light and consequently having no  
 124 need for a high photoprotective capacity). It is important to keep in mind that a momentarily

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125 shaded leaf can actually be sun-adapted and vice versa, depending on its instantaneous and total  
126 diurnal illumination.

127 The implementation of DART chlorophyll fluorescence emission  $F_{xyv}$  (Eq. 2) does not  
128 account for the microclimatic conditions influencing the actual leaf photosynthetic activity.  
129 However,  $F_{xyv}$  can be in a vertical canopy profile additionally weighted by an *eta* parameter,  
130 which adjusts the leaf SIF exitance according to actual local temperature, humidity, wind  
131 aerodynamics and other microclimatic environmental conditions. Similar to *fqe*, the *eta* profile  
132 can be inserted either for a whole canopy, per a foliage group, or per pre-defined leaf groups.  
133 Since DART modelling does not contain soil-vegetation-atmosphere transfer (SVAT) of  
134 energy, the *eta* parameter must be precomputed out of DART with a SVAT model (e.g.,  
135 SCOPE; van der Tol et al. 2009) that considers dynamic meteorological factors as active parts  
136 in computation of the energy balance. DART simulates the total and the per-photosystem  
137  $SIF_{TOC}$  radiance and TOC reflectance using the N-flux tracking transfer. Technical details about  
138 the SIF flux tracking in DART are available in the DART User's Manual (Chapter III.2.2.d;  
139 DART 2020), while DART physical principles and mathematical descriptions are detailed in  
140 the DART Handbook (DART 2019).

### 141 **2.2 Comparison of DART and SCOPE/mSCOPE SIF radiative transfers**

142 In absence of a suitable empirical verification data, we compared the DART  $SIF_{TOC}$  signal  
143 with comparable outcomes produced by the SCOPE model and its multi-layer extension,  
144 mSCOPE (both in version 1.62). SCOPE is a broadly accepted model that has been previously  
145 confronted and validated with  $SIF_{TOC}$  measurements of agricultural crops (van der Tol et al.  
146 2016). It simulates vegetation canopy as a turbid medium of infinitely small leaves distributed  
147 in 60 horizontally homogeneous vertical layers (Yang et al. 2017), all of them with the same  
148 predefined leaf biochemical and canopy structural parameters. mSCOPE allows users to divide  
149 canopy into multiple horizontal layers and to assign to each one specific leaf optical properties  
150 and LAI. The methodology and graphical outputs of the DART and SCOPE/mSCOPE SIF  
151 radiative transfer comparison are, due to a large extent, provided in Appendix A.

### 152 **2.3 DART modelled influence of geometrically explicit plant canopy structures on SIF**

153 DART works with detailed and spatially explicit 3D representations of plant foliage and  
154 other canopy elements (e.g., trunks and branches), and can be, therefore, used to investigate  
155 how the structural components modulate the simulated  $SIF_{TOC}$  signal through optical photon

156 interactions as well as via foliage shading and physiological adaptations to prevailing  
 157 photosynthetic light intensity. For this purpose, we built two realistic but structurally different  
 158 mono-species canopies: i) an agricultural field of 1 m tall maize plants with eight leaves, created  
 159 with the open source graphical software Blender (Blender 2007) according to a template  
 160 produced by the plant architecture modelling L-system OpenAlea (Pradal et al. 2008), and ii) a  
 161 16 m tall forest stand of white peppermint trees, created from terrestrial laser scans of real trees  
 162 (Janoutová et al. 2019) growing in southern Tasmania (Australia). 3D landscapes were built as  
 163 juxtaposed scenes located at the same Latitude of 39.03°N and Longitude of 76.85°W  
 164 (Maryland, USA) as previous simulations, with the solar angles for 10<sup>th</sup> July 2014 for the test  
 165 of foliage sun and shade adaptation and for 26<sup>th</sup> August 2014 at 14.00 of local time (without the  
 166 daylight saving) for tests of maize canopy clumping and eucalypt wood influence. All canopies  
 167 were illuminated by the same DART-simulated BOA direct and diffuse solar irradiance, as  
 168 described in the previous section 2.2. Ground of the 3D scenes was optically defined as the  
 169 Lambertian loamy gravel brown dark soil with a linearly increasing reflectance ( $\rho \approx 6\%$  at 550  
 170 nm,  $\rho \approx 12\%$  at 686 nm and  $\rho \approx 15\%$  at 740 nm).

### 171 2.3.1 Distinction and influence of sun- and shade-adapted foliage in maize crops

172 As explained by Nobel (1976) or Givnish (1988), leaves growing in a shaded environment  
 173 are biochemically and anatomically different from those exposed for most of the day to direct  
 174 solar irradiation. DART users can consider these differences and their influence on SIF<sub>TOC</sub> by  
 175 classifying the facets of 3D vegetation leaves in several classes, for which leaf optical or  
 176 biochemical properties (including *fqe* and *eta* parameters) can be defined separately. The final  
 177 number of classes depends on the structural complexity of canopies and the availability of  
 178 measurements to support the detailed foliar parameterization. A simple two-class classification  
 179 would split leaf facets into just sun- and shade-adapted cohorts (DART 2020), considering a  
 180 long-term cumulative leave irradiance as the main driving force.

181 DART calculates intercepted, absorbed, reflected and emitted radiation, i.e. radiative  
 182 budget, per 3D cell of the simulated scene and also for each surface facet in the scene (Gastellu-  
 183 Etchegorry 2008), which can be used to distinguish between the sun- and shade-adapted leaf  
 184 cohorts. The intercepted radiation flux  $E(\lambda)$  [ $\text{W}\cdot\text{m}^{-2}$ ] can be converted into photosynthetic  
 185 photon flux density Q (PPFD) [ $\mu\text{mol}\cdot\text{photons}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ ] by integrating the intercepted PAR  
 186 (iPAR) per leaf facet as follows:

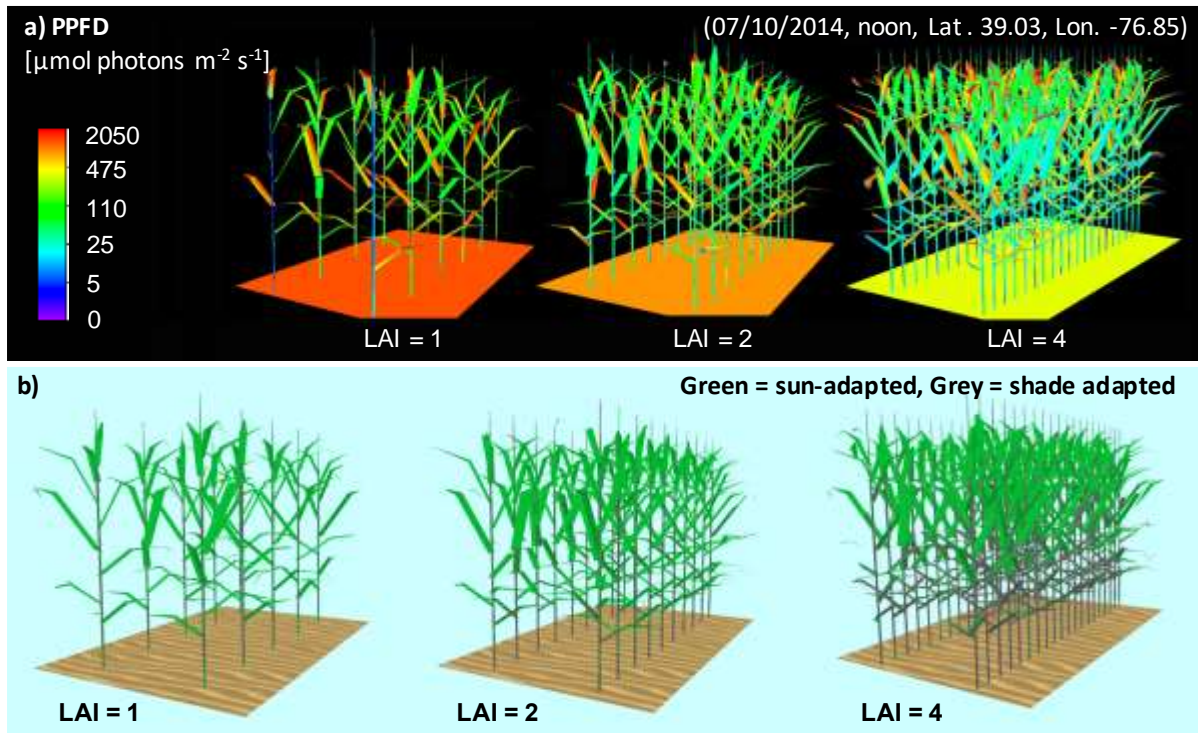
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$$187 \quad Q = \int_{\Delta\lambda_i} E(\lambda) \cdot d\lambda \cdot \frac{\int_{0.4\mu m}^{0.75\mu m} L_B(T, \lambda) \cdot \frac{\lambda \cdot 10^6}{h \cdot c \cdot N_a} \cdot d\lambda}{\int_{0.4\mu m}^{0.75\mu m} L_B(T, \lambda) \cdot d\lambda}, \quad (5)$$

188 where  $L_B(T, \lambda)$  is Planck's law at temperature  $T$  ( $T = 5800$  K) and wavelength  $\lambda$  [ $\mu\text{m}$ ],  $h$  is  
 189 Planck's constant [ $\text{J}\cdot\text{s}$ ],  $c$  is speed of light [ $\text{m}\cdot\text{s}^{-1}$ ],  $N_a$  is Avogadro's constant [ $\text{mole}^{-1}$ ], and  $\int_{\Delta\lambda_i}$   
 190 is the PAR spectral range from 400 to 750 nm. The  $Q$  value depends on the ratio of direct and  
 191 diffuse irradiance spectrum, leaf optical properties and PAR multiple scattering. Influenced by  
 192 literature findings about the potential of  $Q$  for differentiating sun- and shade-adapted leaves  
 193 (Leuning et al. 1995; Niinemets et al. 2015), the following two classification algorithms were  
 194 designed: i) a frequency double-threshold and ii) a probability distribution approach. Both  
 195 methods are based on simulated leaf PAR irradiance values for  $T$  time steps during  $i$  days, with  
 196  $T$  being small enough to ensure an adequate angular sampling of leaf irradiance variation during  
 197 the simulated days.

198 The first double-threshold approach asks user to specify high  $Q_H$  and low  $Q_L$  classification  
 199 thresholds. The facets are then categorized at each time step  $T$  into the three groups: i)  $H$  for  
 200  $Q > Q_H$ , ii)  $L$  for  $Q < Q_L$ , and iii)  $M$  for  $Q_H > Q > Q_L$ . The number of occasions when a leaf  
 201 facet appeared in each of these groups during the simulated day  $i$  is counted, resulting in  $[N_{H,i},$   
 202  $N_{M,i}, N_{L,i}]$  with  $N_{H,i} + N_{M,i} + N_{L,i} = T$ . Subsequently, a leaf facet is labelled as sun-adapted  
 203 (i.e.,  $C_{f,i} = 1$ , with  $f \in [1, F]$  where  $F$  is the total number of leaf facets) if: i)  $N_{H,i} > \frac{T}{2}$  (i.e., leaf  
 204 facet is categorized as sunlit for the majority of the  $T$  time steps), or ii)  $N_{M,i} > \frac{T}{2}$  and  $N_{H,i} >$   
 205  $N_{L,i}$  (i.e., leaf irradiance is, for the majority of  $T$  time steps, between the two thresholds and a  
 206 leaf facet is categorized as sunlit more frequently than shaded). Finally, a leaf facet is labelled  
 207 as shade-adapted (i.e.,  $C_{f,i} = 0$ ) in all other cases, which cover the following three conditions:  
 208 i)  $N_{L,i} > \frac{T}{2}$ , ii)  $N_{M,i} > \frac{T}{2}$  and  $N_{H,i} < N_{L,i}$ , and iii) none of the  $[N_{H,i}, N_{M,i}, N_{L,i}]$  values dominates  
 209 during the simulated times. This way, a day series (an array of  $i$  values) of sun-adapted ( $C_{f,i} =$   
 210 1) and shade-adapted ( $C_{f,i} = 0$ ) states is generated per leaf facet  $f$ . The final class assignment  
 211 is decided based on the median value of  $C_f$  across the entire examined time period.





212

213 Figure 1. Incident photosynthetically active radiation expressed in photosynthetic photon flux density  
 214 (PPFD) for three realistic 3D maize (*Zea mays L.*) canopies with LAI equal to 1, 2 and 4 (a). Distinction  
 215 of sun- (green) and shade- (grey) adapted foliage based on double PPFD thresholds of 50 and 100  
 216  $\mu\text{mol.photons.m}^{-2}.\text{s}^{-1}$  (b). To mimic realistic maize canopies, all three maize fields (1x1.5 m in size)  
 217 were created with 1 m tall semi-randomly oriented plants, having eight fully developed bifacial leaves.  
 218

218

219 The second method uses the probability distribution of the simulated diurnal Q time series.  
 220 The range of Q values is divided into equally or unequally distributed X intervals, and the Q  
 221 values of leaf facets simulated at each time step T are categorized in a group x ( $x \in [1, X]$ ). The  
 222 probability distribution functions of  $i \cdot T$  sampling points are then computed over x groups,  
 223 resulting in the maximum occurrence (i.e., the highest probability density) in group  $x_{\text{max}}$  and  
 224 the median occurrence in group  $x_{\text{median}}$ . A leaf facet is assigned as sun-adapted if  $x_{\text{max}} > \frac{x}{3}$   
 225 and  $x_{\text{max}} \leq x_{\text{median}}$ , and shade-adapted in all other cases. Both methods are available in the  
 226 DART toolbox directory as Python scripts, the decision which to use is solely of user discretion.  
 227

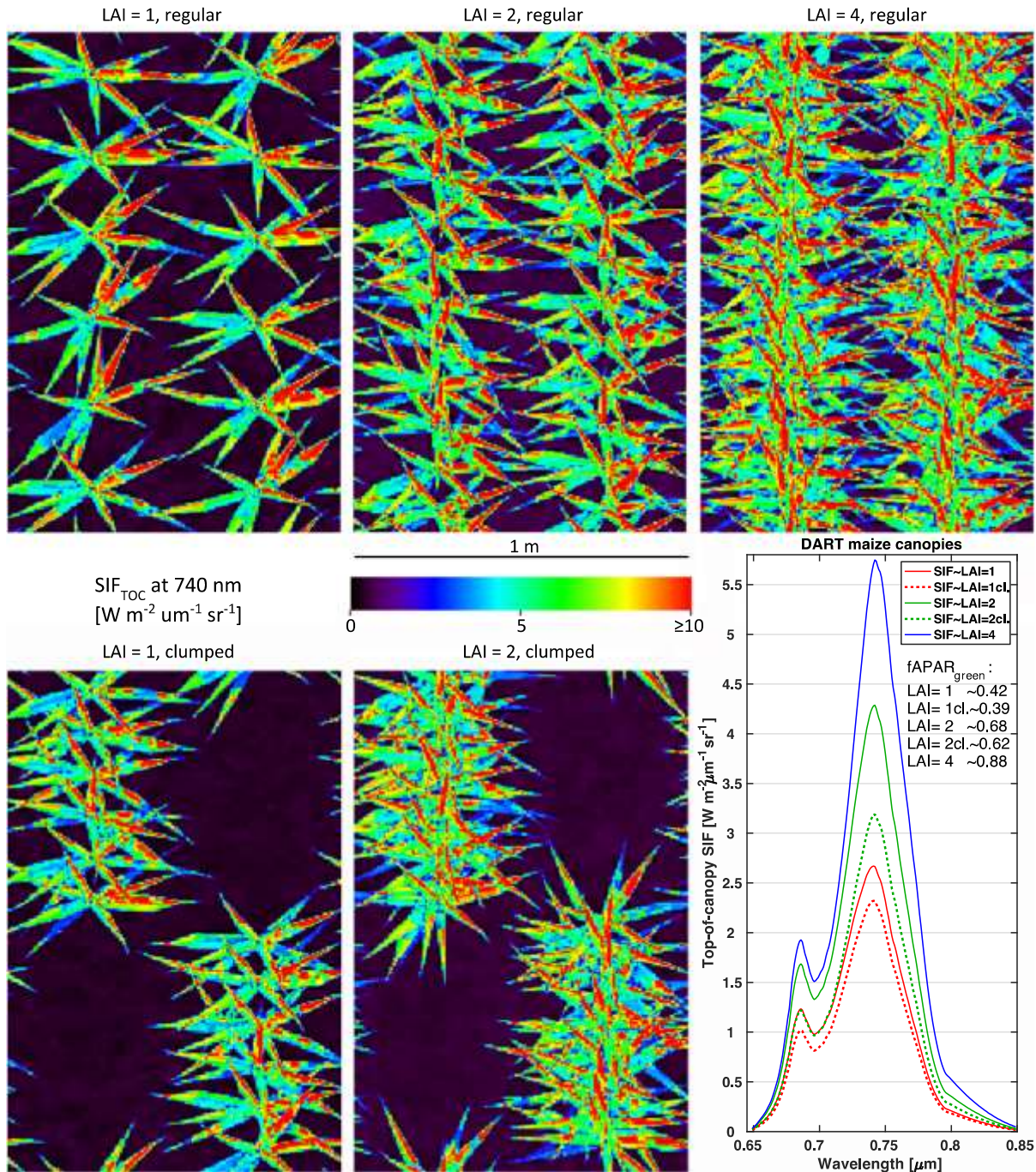
228 To demonstrate changes in SIF<sub>TOC</sub> due to the distinction of sun- and shade-adapted leaves,  
 229 we applied two double-threshold classifications on three maize fields (Figure 1). The first  
 230 ‘relaxed’ classification used relatively high and far-apart thresholds of 50 and 100  
 231  $\mu\text{mol.photons.m}^{-2}.\text{s}^{-1}$ , allowing for a larger portion of shade-adapted parts, whereas the second  
 232 ‘strict’ classification used low and close thresholds of 15 and 25  $\mu\text{mol.photons.m}^{-2}.\text{s}^{-1}$ , resulting  
 in a smaller amount of strictly shade-adapted leaves and stems. The regularly spaced 1 m tall

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233 plants with fully developed bifacial leaves were placed in fields (1x1.5 m in size) with a random  
 234 geographical orientation and distances resulting in LAI = 1, 2 and 4. Specific leaf biochemical,  
 235 structural and fluorescence properties were assigned to each leaf adaptation class as listed in  
 236 Table 1 (note that foliage of scenarios without distinct light adaptations was assumed to have  
 237 the properties of sun-adapted leaves and stems). Contrary to previous SIF simulations, PSII *fqe*  
 238 values of medium magnitude were assigned to each leaf class, while PSI *fqe* values were kept  
 239 constant under the assumption that PSI contributes to SIF signal of both leaf types equally (Liu  
 240 et al. 2019a). In order to prevent its confounding effect, the energy balance (leaf photosynthesis)  
 241 modelling was disregarded, i.e., the fluorescence efficiency weight *eta* was forced to one. The  
 242 remaining inputs were arbitrarily defined within plausible dynamic ranges of published  
 243 laboratory measurements (Hosgood et al. 1994; Jacquemoud and Baret 1990).

244 Table 1. Input parameters of the Fluspect-Cx model to simulate optical properties of sun- and shade-  
 245 adapted leaves, as well as foliage without light adaptations and stems: content of chlorophyll *a+b* (Cab),  
 246 total content of carotenoids (Car), equivalent water thickness (EWT), leaf mass per area (LMA),  
 247 mesophyll optical thickness number (N) and fluorescence quantum efficiencies (*fqe*) for PSI and PSII.

Fluspect inputs	Cab [ $\mu\text{g}\cdot\text{cm}^{-2}$ ]	Car [ $\mu\text{g}\cdot\text{cm}^{-2}$ ]	EWT [cm]	LMA [ $\text{g}\cdot\text{cm}^{-2}$ ]	N	PSI <i>fqe</i>	PSII <i>fqe</i>
Sun-adapted and without adaptation leaves and stems	50	15	0.009	0.0021	1.5	0.002	0.016
Shade-adapted leaves and stems	75	20	0.012	0.0028	2.0	0.002	0.022



248

249 Figure 2. DART simulated images of top-of-canopy SIF at 740 nm for maize fields of three leaf area  
 250 indices (LAI) and two canopy closures, 100% regular (top) and 50% clumped (bottom), given by the  
 251 number of plants (LAI = 1 ~ 12 plants, LAI = 1 ~ 24 plants and LAI = 4 ~ 50 plants) associated with  
 252 different plant distances. The graph (bottom-right) displays the corresponding modelled canopy SIF  
 253 spectra between 650 and 850 nm and provides the fAPAR<sub>green</sub> values per scenario.

254 *2.3.2 Canopy SIF changes due to leaf density and clumping of maize plants*

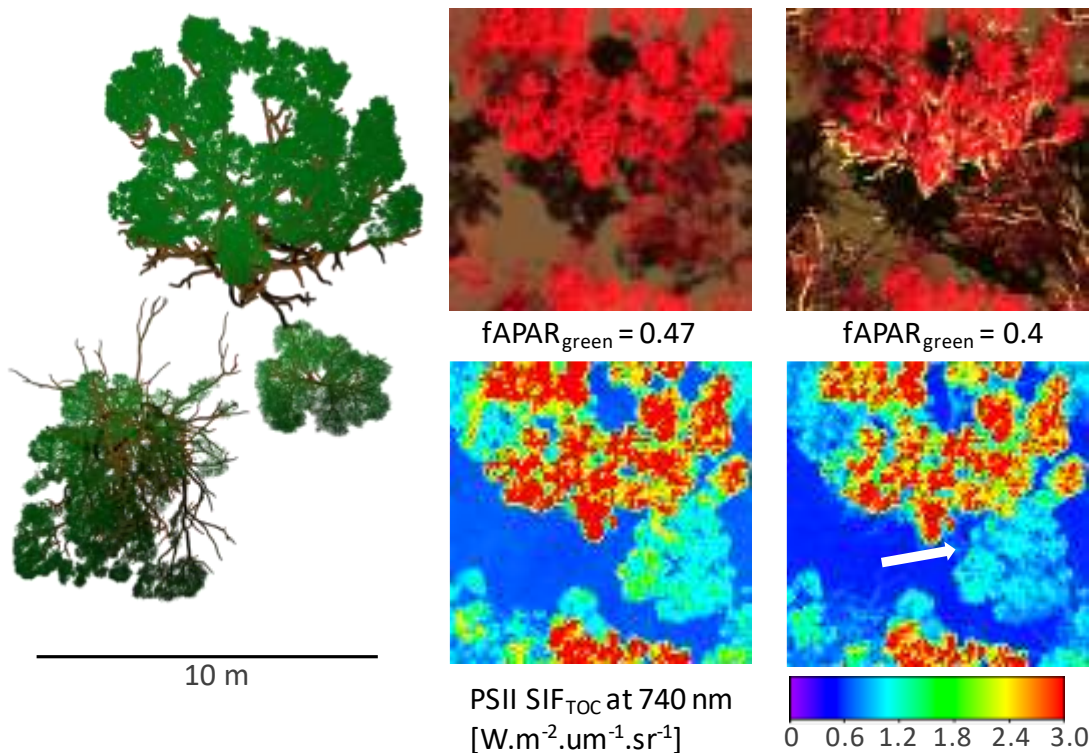
255 Potential variability in SIF<sub>TOC</sub> due to leaf density and plant clumping (i.e., canopy closure  
 256 – CC) changes were simulated for virtual maize canopies of three plant densities (LAI = 1, 2



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257 and 4) in a regular spatial distribution ( $CC \approx 100\%$ ) and in two clumped formations (LAI = 1  
258 and 2,  $CC \approx 50\%$ ) (Figure 2). Compared to the previous exercise (Figure 1), distances between  
259 6 (LAI = 1) or 12 (LAI = 2) of neighbouring regularly spaced plants in a row were shortened  
260 by half to create regular foliage clumps and canopy gaps of the same size. To keep consistency,  
261 the leaf and stem optical properties were those used for the turbid-like canopies (Table A1) and  
262 the sun- and shade-adaptations were not distinguished, i.e., all leaves were considered as equal.

a) 3D forest stand representation    b) Canopy of only foliage    c) Canopy with wood



263

264 Figure 3. Nadir view of 3D representation of the dense white peppermint (*Eucalyptus pulchella*) test  
265 canopy derived from terrestrial laser scans of trees growing east of Hobart (Tasmania, Australia) (a).  
266 The virtual scene (LAI = 2) was used to simulate a near-infrared, red and green RGB false colour  
267 composite images in DART of top-of-canopy reflectance (top) as well as PSII SIF at 740 nm (bottom)  
268 of the canopy formed by: b) only foliage and c) foliage and woody material covered with bark. The  
269 white arrow points at the example of SIF reflection from an exposed tree branch surface.

### 270 2.3.3 Influence of leaf clumping, trunks and branches on SIF of white peppermint canopies

271 DART simulations of eucalyptus forest canopies were used to investigate potential impacts  
272 of leaf clumping and woody material, i.e., trunks and branches covered by bark, on SIF<sub>TOC</sub>  
273 modelled at 686 and 740 nm. 3D representations of the eucalyptus trees were constructed based  
274 on 3D point clouds acquired with the terrestrial laser scanner (TLS) Trimble TX8 (Trimble Inc.,  
275 USA). Three native white peppermint eucalypts of different age, height and general habitus

276 were scanned from several geolocations in dry sclerophyll forest located southeast of Hobart  
 277 (Tasmania, Australia) to acquire their TLS point clouds with a point spacing of 11.3 mm at  
 278 distance of 30 m. The TLS points of each tree were, after a mandatory pre-processing, semi-  
 279 automatically separated in two groups: i) points of trunks and branches and ii) points  
 280 representing foliage. Points classified as wood were used as attractors in an automatic procedure  
 281 (Sloup 2013) to extract the external surfaces of trunks and main branches, as described in  
 282 Verroust and Lazarus (1999). The foliage points were subsequently spatially collocated with  
 283 the reconstructed wooden skeleton. 3D representation of leaves was created in Blender (Blender  
 284 2007) based on an average shape and size of actual leaves and then distributed automatically at  
 285 the locations of foliage points according to the Erectophile LAD (Danson 1998), targeting two  
 286 crown LAI values of 2 and 5. A complete description of this TLS-based 3D construction of  
 287 trees, developed specifically for RTM purposes, is available in Janoutová et al. (2019). Two  
 288 DART canopies (scenes), were constructed with the 3D tree representations: i) a dense canopy  
 289 was created by placing three trees with the individual crown LAI = 2 within a scene of 81 m<sup>2</sup>,  
 290 while keeping CC ≈ 80% (Figure 3a), and ii) a sparse canopy was built by redistributing the  
 291 same trees but with the crown LAI = 5 within a scene of 196 m<sup>2</sup> to achieve CC ≈ 40%.  
 292 Combinations of the tree crown LAI and scene sizes ensured that both scenes had, for the  
 293 purpose of comparability, the same canopy LAI = 2.5. Additionally, an identical bark  
 294 directional-hemispherical reflectance ( $\rho \approx 20\%$  at 550 nm,  $\rho \approx 40\%$  at 686 nm and  $\rho \approx 50\%$  at  
 295 740 nm), measured on actual bark samples collected in field, was applied in both canopies.

296 Besides standard forest canopies (e.g., Figure 3c), the virtual environment of the DART  
 297 model also allows for simulating canopies composed of only foliage without woody  
 298 components (Figure 3b). By comparing results from simulations with and without woody  
 299 material, we quantified the magnitudes of shading and direct obstructing effects of woody  
 300 material. Removing woody components increases the within-canopy iPAR (Q) due to the  
 301 reduction in wood shadowing, which in turn increases SIF emitted by all previously shaded  
 302 leaves. The obstruction impact of woody material is caused by its optical interactions with SIF  
 303 photons. First, it diminishes (blocks) the within-canopy SIF at both 686 and 740 nm via bark  
 304 scattering and absorption. Second, it affects, to some extent, SIF emission through reflection of  
 305 SIF at 686 nm that can be reabsorbed and later reemitted by chlorophyll pigments.

#### 306 **2.4 Computation of canopy $fAPAR_{green}$ , SIF balance, escape factors and differences**

## 2.1 VEGETATION SIMULATED AS FACETS

307 The main driver of green foliage SIF emissions (including stems of the maize plants) in  
 308 DART simulations that do not contain a modulation of PSI and PSII *fqe* values by *eta*  
 309 coefficients is the fraction of absorbed photosynthetically active radiation ( $fAPAR_{green}$ ).  
 310 Therefore, a change of  $fAPAR_{green}$  in these simulations indicates a change in the ratio of sunlit  
 311 and shaded photosynthetically active plant parts, which results in an equal relative change in  
 312 SIF leaf emission of both photosystems. To be able to investigate the impact of different 3D  
 313 canopy architectures on their  $fAPAR_{green}$ , we calculated  $fAPAR_{green}$  for all SIF<sub>TOC</sub> simulating  
 314 scenarios from the DART radiative budget of a single broad PAR band ( $\lambda = [400\ 750]$  nm) as:

$$315 \quad fAPAR(\lambda)_{green} = \frac{APAR(\lambda)_{green}}{PAR(\lambda)_{TOC}}, \quad (6)$$

316 where  $APAR(\lambda)_{green}$  is PAR absorbed by all green plant constituents of a given DART scene  
 317 and  $PAR(\lambda)_{TOC}$  is the solar incoming PAR simulated at the top of canopy. The relative  
 318 difference [%] in  $fAPAR_{green}$  of clumped (C) compared to regularly spaced (R) maize canopies  
 319 was calculated as:

$$320 \quad \varepsilon_{fAPAR(\lambda)} = 100 \cdot \frac{fAPAR(\lambda)_{green\_C} - fAPAR(\lambda)_{green\_R}}{fAPAR(\lambda)_{green\_R}}. \quad (7)$$

321 Similarly, the shading effect of woody components on eucalyptus SIF emissions was assessed  
 322 through the relative difference [%] of canopy  $fAPAR_{green}$  obtained for simulations containing  
 323 just foliage (F) and foliage with wood (FW) as follows:

$$324 \quad \varepsilon_{fAPAR(\lambda)} = 100 \cdot \frac{fAPAR(\lambda)_{green\_F} - fAPAR(\lambda)_{green\_FW}}{fAPAR(\lambda)_{green\_FW}}. \quad (8)$$

325 DART-simulated 3D radiative budget of SIF allows for locating origins of remotely sensed  
 326 SIF using the SIF balance ( $SIF(\lambda)_{bal}$ ) [ $W \cdot m^{-2} \cdot \mu m^{-1}$ ], computed by subtracting the absorbed SIF  
 327 flux from the total emitted SIF flux (i.e.,  $SIF(\lambda)_{PSI}$  plus  $SIF(\lambda)_{PSII}$ ) of a given wavelength ( $\lambda$ )  
 328 per a vertical canopy layer. A positive  $SIF(\lambda)_{bal}$  means that the canopy layer acts as a SIF source,  
 329 while a negative  $SIF(\lambda)_{bal}$  indicates canopy parts acting as SIF sinks. Subsequently, relative  
 330 difference [%] of  $SIF(\lambda)_{bal}$  between clumped (C) and regularly spaced (R) maize canopies,  
 331 computed as:

$$332 \quad \varepsilon_{SIF(\lambda)_{bal}} = 100 \cdot \frac{SIF(\lambda)_{bal\_C} - SIF(\lambda)_{bal\_R}}{SIF(\lambda)_{bal\_R}}, \quad (9)$$

333 reveals if the maize foliage clumping causes a further reduction ( $\varepsilon_{SIF(\lambda)_{bal}} < 0$ ) or an  
 334 enhancement ( $\varepsilon_{SIF(\lambda)_{bal}} > 0$ ) or no change ( $\varepsilon_{SIF(\lambda)_{bal}} = 0$ ) of SIF balance per a canopy layer.

335 The proportion of SIF photons that exit the top of canopy is described by the SIF<sub>TOC</sub> escape  
 336 probability factor (SIF<sub>esc</sub>). In practice, this is the ratio of SIF photons escaping from the top of  
 337 canopy in any direction to all SIF photons emitted from all canopy leaves in forward or  
 338 backward directions (Guanter et al. 2014). SIF<sub>esc</sub> is required for scaling of SIF<sub>TOC</sub> measurements  
 339 down at the spatial level of individual leaves (van der Tol et al. 2019), and subsequently  
 340 essential for correct estimation of vegetation gross primary production (GPP) from airborne and  
 341 spaceborne SIF observations (e.g., He et al. 2017; Zhang et al. 2020). Since most of RS  
 342 observations capture SIF<sub>TOC</sub> from nadir, we computed the relative canopy SIF escape  
 343 probability factor of a given wavelength ( $\lambda$ ) in the nadir direction (SIF<sub>nadir</sub>( $\lambda$ )<sub>esc</sub>) from SIF  
 344 radiative budgets of the eucalyptus scenarios. First, we converted SIF emissions of PSI and PSII  
 345 per m<sup>2</sup> of abaxial and adaxial leaf facets into SIF emissions per m<sup>2</sup> of the scene ( $F(\lambda)_{\text{PSI}}$  and  
 346  $F(\lambda)_{\text{PSII}}$ ) [W.m<sup>-2</sup>. $\mu\text{m}^{-1}$ ] and then calculated SIF<sub>nadir</sub>( $\lambda$ )<sub>esc</sub> as:

$$347 \quad \text{SIF}_{\text{nadir}}(\lambda)_{\text{esc}} = \frac{\pi \cdot (L_{\text{nadir}}(\lambda)_{\text{PSI}} + L_{\text{nadir}}(\lambda)_{\text{PSII}})}{F(\lambda)_{\text{PSI}} + F(\lambda)_{\text{PSII}}}, \quad (10)$$

348 where  $L_{\text{nadir}}(\lambda)_{\text{PSI}}$  and  $L_{\text{nadir}}(\lambda)_{\text{PSII}}$  [W.m<sup>-2</sup>. $\mu\text{m}^{-1}$ .sr<sup>-1</sup>] are DART modelled PSI and PSII SIF  
 349 radiances at the wavelength ( $\lambda$ ), respectively, escaping from the simulated scene in the nadir  
 350 viewing direction. The  $\pi$  multiplication in Eq. 10 is removing the angular dependency [sr<sup>-1</sup>],  
 351 resulting in relative values of SIF<sub>nadir</sub>( $\lambda$ )<sub>esc</sub> between 0 and 1. Since the escape probability factor  
 352 is predominantly dependent on direct optical interactions with canopy elements that attenuate  
 353 an emitted SIF signal, we quantified the obstruction (blocking) effect of eucalyptus woody  
 354 components on canopy SIF in the nadir viewing direction through the relative difference [%]  
 355 of SIF<sub>nadir</sub>( $\lambda$ )<sub>esc</sub>, computed from the foliage only (F) and the foliage with wood (FW)  
 356 simulations as follows:

$$357 \quad \varepsilon_{\text{SIF}(\lambda)_{\text{esc}}} = 100 \cdot \frac{\text{SIF}_{\text{nadir}}(\lambda)_{\text{esc}_F} - \text{SIF}_{\text{nadir}}(\lambda)_{\text{esc}_{FW}}}{\text{SIF}_{\text{nadir}}(\lambda)_{\text{esc}_{FW}}}. \quad (11)$$

358 Finally, to analyse differences in SIF fluxes escaping from individual simulated canopy layers  
 359 in all directions (i.e., towards layers of the upper and lower hemispheres), we computed from  
 360 DART 3D radiative budget their relative omnidirectional escape factor (SIF<sub>omni</sub>( $\lambda$ )<sub>esc</sub>) as:

$$361 \quad \text{SIF}_{\text{omni}}(\lambda)_{\text{esc}} = \frac{(F(\lambda)_{\text{PSI}} + F(\lambda)_{\text{PSII}}) - (A(\lambda)_{\text{PSI}} + A(\lambda)_{\text{PSII}})}{F(\lambda)_{\text{PSI}} + F(\lambda)_{\text{PSII}}}, \quad (12)$$

362 where  $A(\lambda)_{\text{PSI}}$  and  $A(\lambda)_{\text{PSII}}$  [W.m<sup>-2</sup>. $\mu\text{m}^{-1}$ ] are DART modelled absorptances of PSI and PSII SIF,  
 363 respectively, expressed for the wavelength ( $\lambda$ ) per m<sup>2</sup> of the scene. If SIF<sub>omni</sub>( $\lambda$ )<sub>esc</sub>  $\leq$  0, then

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364 the canopy layer does not contribute to the  $SIF_{TOC}$  signal, i.e., its  $SIF(\lambda)_{bal}$  is either neutral or  
365 negative.

### 366 *2.5 DART settings common to all SIF canopy simulations*

367 DART simulations were carried out with the flux-tracking algorithm using the following  
368 settings: no elimination of low energy rays, relative accuracy on scene albedo equal to  $10^{-6}$ , 25  
369 duplications of the initially simulated scene, the scene illumination mesh size equal to  $5 \cdot 10^{-4}$  m  
370 (with a semi-random spatial distribution of illumination rays), and cell sub-sampling with  $8^3$   
371 sub-cells per cell and 1 sub face per cell face. An optimal number of 20 flux-tracking iterations,  
372 which were required to obtain a  $10^{-2}$  relative accuracy of the scene reflectance, was determined  
373 through a simplified accuracy sensitivity study. Intermediate results of the last few iterations  
374 were used to extrapolate the final values of simulated radiative budget, bidirectional reflectance  
375 function and SIF products. TOC reflectance and SIF were simulated in 212 viewing directions  
376 (Yin et al. 2013), distributed systematically throughout the upward hemisphere, with an  
377 oversampling of the upward hot-spot region (25 directions in a solid angle of 0.01 sr around the  
378 hotspot direction) and 34 virtual viewing directions in the solar principle plane. Leaf facets  
379 were simulated as double-faces without the solar penumbra effect, all optical properties were  
380 assumed to be Lambertian, and the scene ground surface was horizontal.

### 381 *2.6 Comparative statistical indicators*

382 Comparative statistical indicators, specifically a root mean square error (RMSE) and an  
383 index of agreement (d), were computed to assess these similarities as well as anticipated  
384 statistical dissimilarities between different DART scenarios (i.e., turbid-like vs. maize and  
385 eucalypt canopies). As explained in Willmott (1981), the dimensionless index of agreement  
386 complements the RMSE by indicating the degree of correspondence between two tested  
387 datasets in magnitude and direction, where  $d = 1$  means full agreement and  $d = 0$  means total  
388 disagreement. Also, the similarity of DART and SCOPE multi-angular  $SIF_{TOC}$  was assessed  
389 through fitting a linear regression model, where the regression coefficient of determination ( $R^2$ )  
390 indicated how much of the variability in a reference RT model (i.e., SCOPE) results can be  
391 explained by corresponding regressed values simulated in DART.

## 392 **3. Results**



### 393 **3.1 Comparison of nadir DART and SCOPE/mSCOPE canopy SIF simulations**

394 The SCOPE and DART nadir SIF<sub>TOC</sub> signatures of turbid medium vegetation canopies  
 395 were nearly identical (Figure A2). Results between 641 and 850 nm were comparable for all  
 396 simulated input combinations (i.e., three LAI, three LAD and three soil types). High SIF<sub>TOC</sub>,  
 397 observed for canopies of Planophile LAD, is caused by their high PAR interception efficiency.  
 398 The highest RMSE = 0.162 W.m<sup>-2</sup>.μm<sup>-1</sup>.sr<sup>-1</sup> and the lowest d = 0.9965 were found for the  
 399 Erectophile canopy of LAI = 1, covering soil with ρ = 50%. Despite being the worst case, the  
 400 values indicate only minor differences between DART and SCOPE results. Statistical analyses  
 401 revealed that the total SIF<sub>TOC</sub> RMSE originates mainly from RMSE for PSII, which was twice  
 402 the RMSE for PSI simulations for all three LADs (results not shown). Despite a significantly  
 403 higher variability in RMSE than other two LADs, the Planophile LAD showed the highest index  
 404 of agreement and R<sup>2</sup> computed between the two models.

405 mSCOPE allowed us to introduce a biochemical/optical heterogeneity in the vertical  
 406 dimension of simulated canopies. Additionally, we tested DART SIF simulation performance  
 407 when using the energy balance *eta* coefficients produced by mSCOPE. Comparison of total  
 408 nadir SIF<sub>TOC</sub> radiances produced by both models revealed almost the same results (Figure A3).  
 409 The indices of agreement were in all cases larger than 0.99, regardless exclusion or inclusion of  
 410 the mSCOPE *eta* coefficients in conducted simulations. The highest RMSE of just 0.221 W.m<sup>-2</sup>.μm<sup>-1</sup>.sr<sup>-1</sup>  
 411 and the lowest d = 0.9985 was found for simulation of 2-layered canopy with LAI =  
 412 2 and with the leaf energy balance included (Figure A3b).

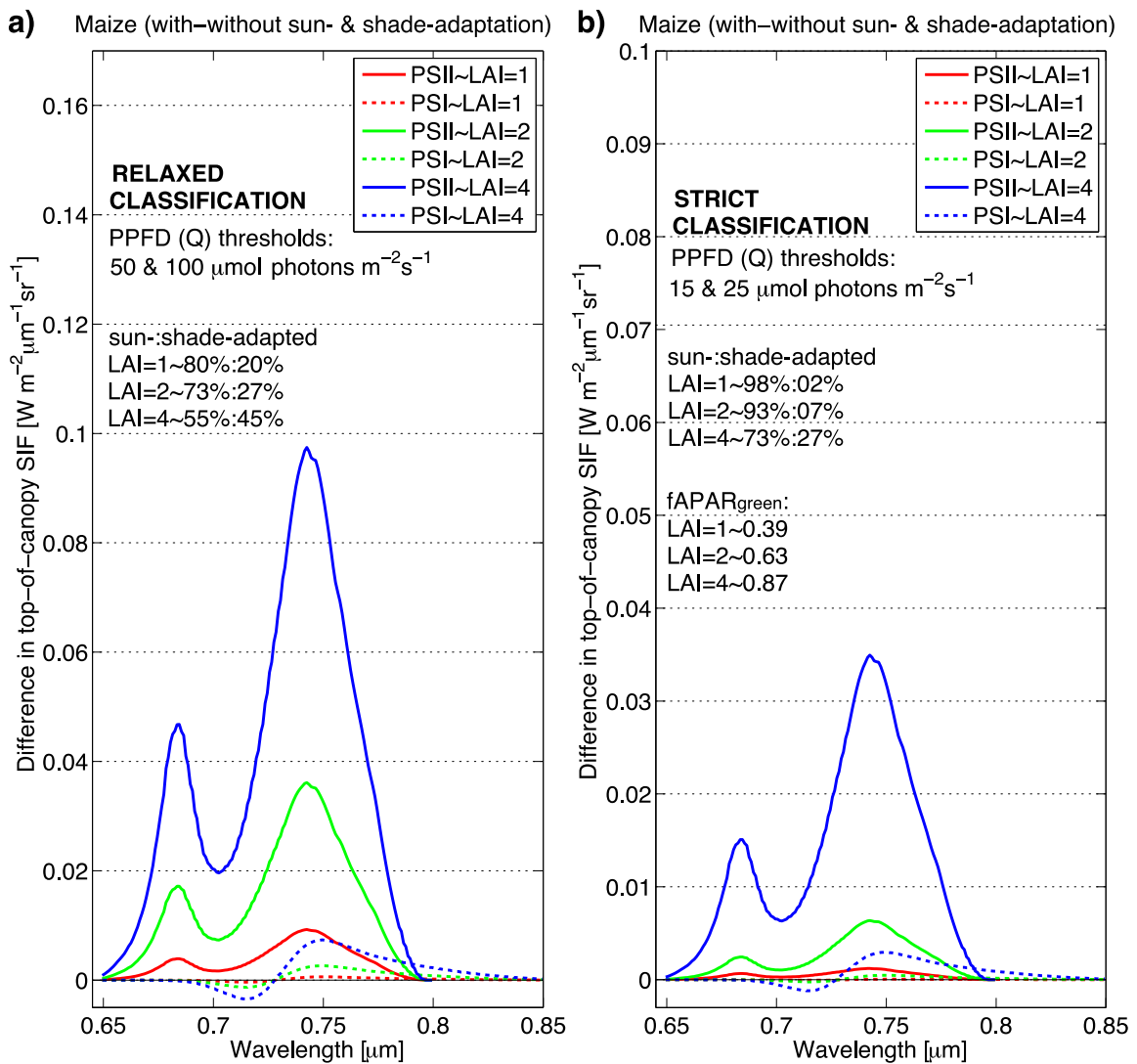
### 413 **3.2 Multi-angular comparison of DART and SCOPE canopy SIF simulations**

414 The similarity of DART and SCOPE SIF<sub>TOC</sub> simulations at 686 and 740 nm was also  
 415 investigated for viewing directions other than the nadir view. We compared values simulated  
 416 in the solar principal plane, with particular attention to the hotspot region, and computed  
 417 absolute differences between 27 DART and SCOPE turbid medium scenarios in all 212 viewing  
 418 directions. The smallest differences and the best agreement were found for SIF<sub>TOC</sub> at 686 nm,  
 419 Erectophile LAD and LAI = 1 (Figure A4), while the worse agreement and largest differences  
 420 were obtained for SIF<sub>TOC</sub> at 740 nm, Spherical LAD and LAI = 4 (Figure A5). Here, SCOPE  
 421 simulated slightly smaller SIF<sub>TOC</sub> values, except for VZA > 75°, where SIF<sub>TOC</sub> dropped  
 422 unexpectedly steeply down. Also, SCOPE values around the hotspot angles were about 1 W.m<sup>-2</sup>

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423  $^2 \cdot \mu\text{m}^{-1} \cdot \text{sr}^{-1}$  lower than the corresponding DART values. This is caused by differences in the  
 424 vegetation hotspot algorithms. SCOPE uses a Kuusk's analytical approximation, which does  
 425 not account for a bi-directional gap-fraction correlation with the canopy depth and consequently  
 426 underestimates the hotspot effect (Kallel and Nilson 2013), whereas hotspot in DART  
 427 simulations is physically modelled.

428 Analysis of multi-angular SIF differences among the three LADs stressed smaller  
 429 dissimilarities at 686 nm, having the best fit for the Spherical LAD, followed by the Erectophile  
 430 LAD, and then by the Planophile LAD. At 740 nm, the closest match occurred for the  
 431 Planophile LAD, while the Spherical and the Erectophile LADs showed equal discrepancies  
 432 (Figure A6). Nonetheless, the maximal absolute SIF<sub>TOC</sub> difference between DART and SCOPE  
 433 oblique viewing directions of all scenarios was found to be  $< 0.8 \text{ W} \cdot \text{m}^{-2} \cdot \mu\text{m}^{-1} \cdot \text{sr}^{-1}$ .



434

435 Figure 4. Differences in DART top-of-canopy SIF radiance due to distinction of sun- and shade-adapted  
 436 leaves of regular maize canopies with LAI = 1, 2 and 4. Graphs illustrate two simulated scenarios of  
 437 photosynthetic photon flux density (PPFD or Q) classification thresholds: a) a ‘relaxed’ scenario with  
 438 high PPFD thresholds of 50 and 100  $\mu\text{mol.photons.m}^{-2}.\text{s}^{-1}$ , and b) a ‘strict’ scenario with low PPFD  
 439 thresholds of 10 and 25  $\mu\text{mol.photons.m}^{-2}.\text{s}^{-1}$ . For details about the double-threshold leaf light adaptation  
 440 classification see section 2.3.1.

### 441 **3.3 Effect of sun- and shade-adapted maize foliage classification**

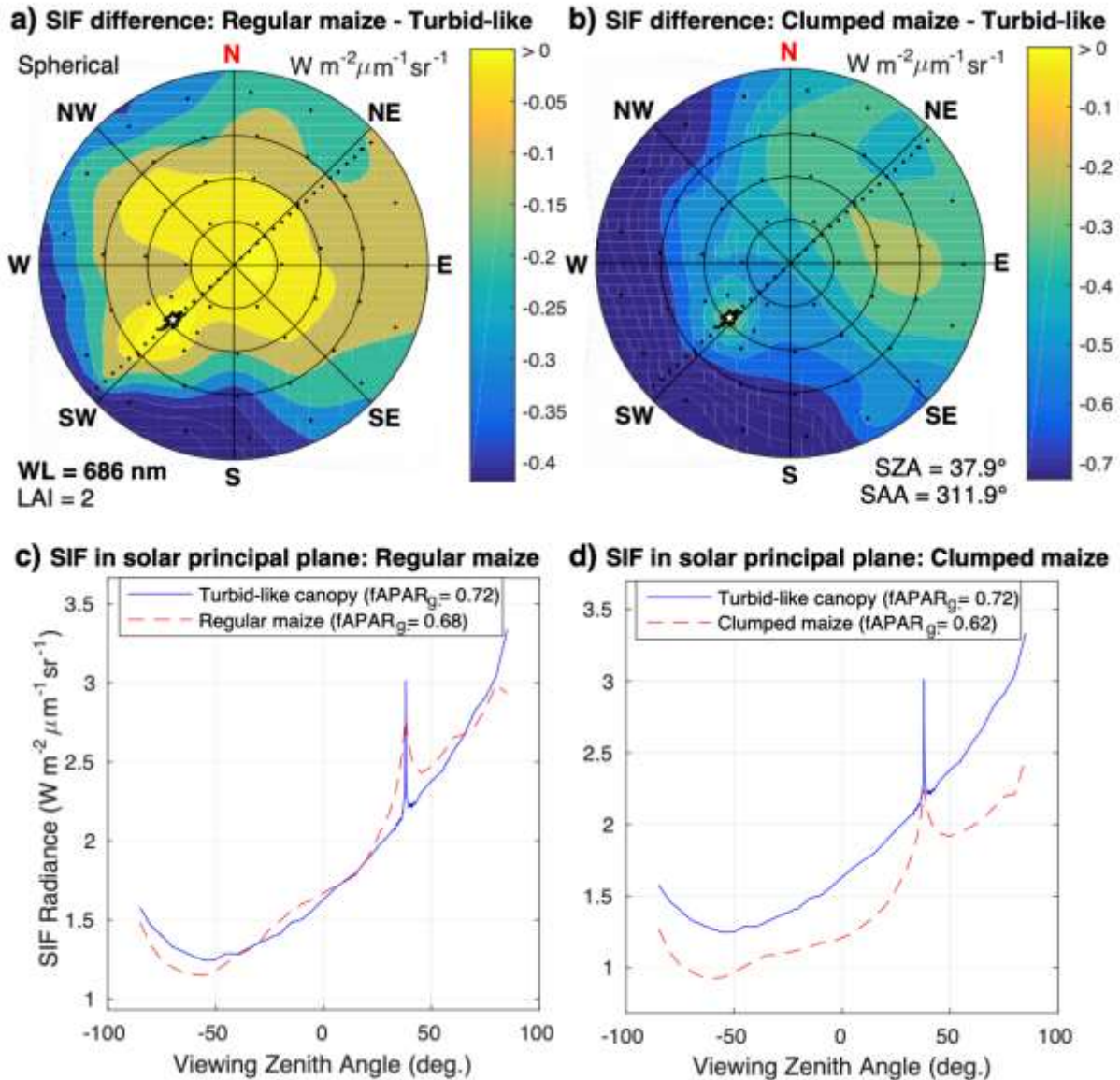
442 Two double-threshold classifications were used to assess the impact of sun- and shade-  
 443 adapted foliage differentiation on nadir PSI and PSII SIF<sub>TOC</sub> between 650-850 nm. The first  
 444 one, called ‘relaxed’, used the far-apart high Q thresholds (50 and 100  $\mu\text{mol.photons.m}^{-2}.\text{s}^{-1}$ ),  
 445 resulting in the sun-to-shade adapted foliage ratio ranging from 80:20% (LAI = 1) to 55:45%  
 446 (LAI = 4). Figure 4a shows that differences between SIF<sub>TOC</sub> signatures for simulations with and  
 447 without the differentiation of sun-/shade-adapted leaves were all positive for PSII, with the  
 448 highest value  $\approx 0.1 \text{ W.m}^{-2}.\mu\text{m}^{-1}.\text{sr}^{-1}$  around 740 nm for LAI = 4 ( $f\text{APAR}_{\text{green}} = 0.87$ ). Surprisingly,  
 449 the same differences for PSI between 700 and 725 nm were negative, demonstrating a greater  
 450 PSI SIF absorption by shade-adapted leaves having a higher chlorophyll *a+b* content of 75  
 451  $\mu\text{g.cm}^{-2}$ . Contrary to PSII SIF<sub>TOC</sub>, where *fqe* was increased from 0.016 to 0.022 for shade-  
 452 adapted leaves (Table 2), the constant PSI *fqe* of 0.002 could not compensate this increased  
 453 chlorophyll absorption. The second classification, called ‘strict’, used the closer and lower Q  
 454 thresholds (15 and 25  $\mu\text{mol.photons.m}^{-2}.\text{s}^{-1}$ ), resulting in canopies with a dominant portion of  
 455 sun-adapted leaves. The sun-to-shade adapted foliage ratio ranged from 98:2% (LAI = 1) to  
 456 73:27% (LAI = 4). Consequently, the SIF<sub>TOC</sub> differences were proportionally smaller (Figure  
 457 4b), with the largest value of 0.035  $\text{W.m}^{-2}.\mu\text{m}^{-1}.\text{sr}^{-1}$  for PSII SIF<sub>TOC</sub> at 740 nm (LAI = 4). PSI  
 458 SIF<sub>TOC</sub> differences were also reduced and remained negative between 700 and 725 nm.

### 459 **3.4 Influence of foliage density and clumping in maize canopies**

460 Figure 2 illustrates the impact of a leaf density increase (i.e., doubled LAI) and the  
 461 clumping of maize plants for LAI of 1 and 2. Nadir images of maize canopy SIF<sub>TOC</sub> at 740 nm  
 462 show the spatial dependence of SIF<sub>TOC</sub> radiance on the absorption of iPAR and on the  
 463 distribution of plant shadows. A linear increase of LAI triggered a non-linear and wavelength-  
 464 specific increase of SIF<sub>TOC</sub>. A bit more than 2-fold increase in far-red wavelengths from LAI =  
 465 1 to LAI = 4 corresponds to a similar increase in canopy  $f\text{APAR}_{\text{green}}$ , which is not the case for  
 466 the red SIF<sub>TOC</sub> nadir signal (Figure 2). The canopy clumping causes a decrease of SIF<sub>TOC</sub> at all

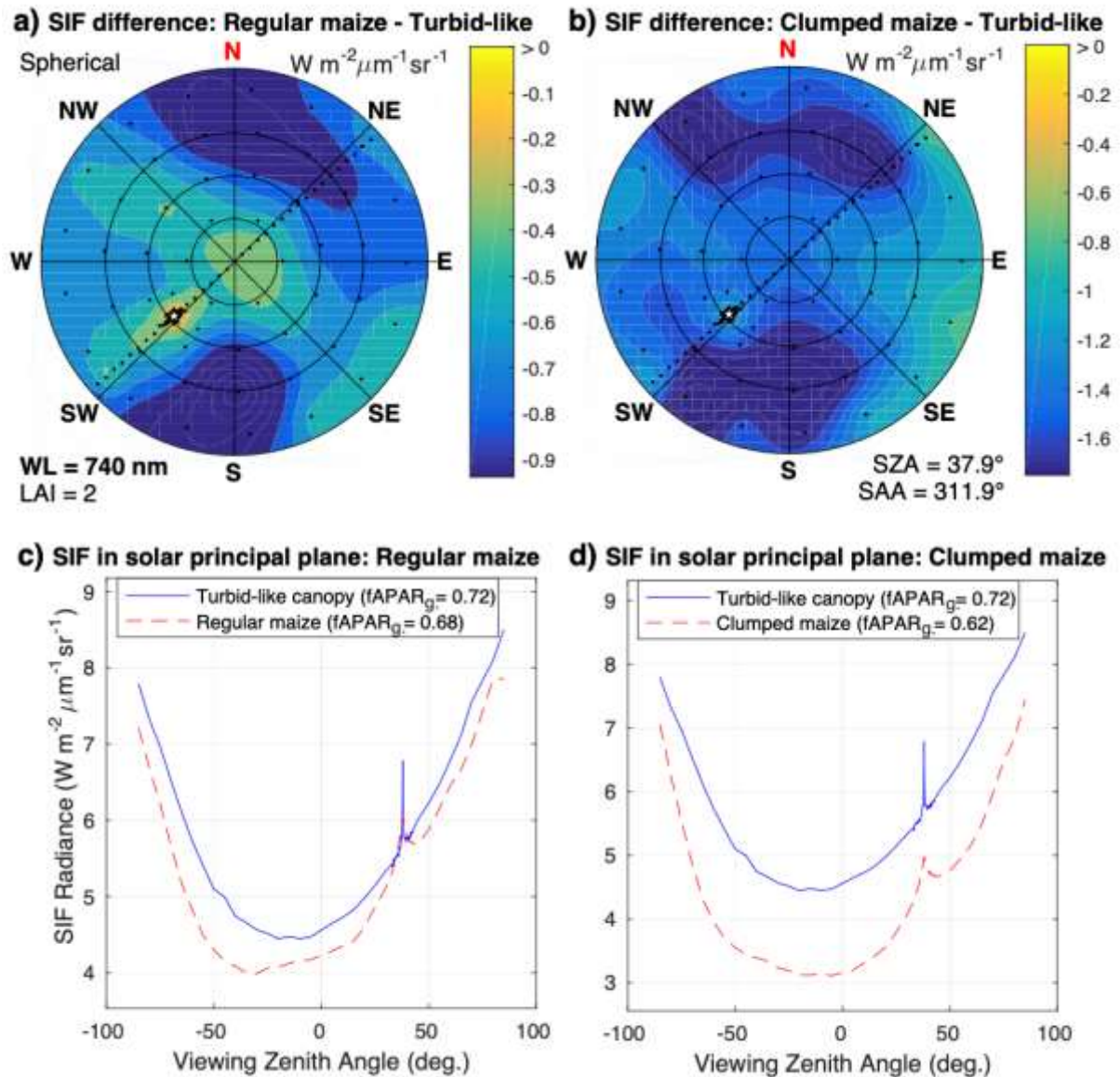
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467 wavelengths. The 50% decrease in CC caused SIF<sub>TOC</sub> reduction at 740 nm of about 0.4 for LAI  
 468 = 1 and 1.0  $W \cdot m^{-2} \cdot \mu m^{-1} \cdot sr^{-1}$  for LAI = 2, whereas reduction of LAI from 2 to 1 resulted in larger  
 469 SIF<sub>TOC</sub> declines of about 0.75 for CC = 50% and 1.6  $W \cdot m^{-2} \cdot \mu m^{-1} \cdot sr^{-1}$  for CC = 100%.



470

471 Figure 5. Multi-angular differences in SIF radiance at 686 nm between a) regular, b) clumped DART  
 472 3D maize canopies and a DART simulated turbid-like canopy with LAI = 2, Spherical LAD and loamy  
 473 soil as ground. SIF radiances in the solar principal plane for the turbid-like canopy together with the  
 474 regular (RMSE = 0.27 and d = 0.9) and the clumped (RMSE = 0.36 and d = 0.81) maize canopies are  
 475 illustrated in c) and d), respectively. Notations: the white star shows the solar position and black dots  
 476 indicate the simulated viewing directions; LAD ~ leaf angle distribution; LAI ~ leaf area index; WL ~  
 477 wavelength; SZA ~ solar zenith angle; SAA ~ solar azimuth angle; R<sup>2</sup> ~ coefficient of determination;  
 478 RMSE ~ root mean square error [ $W \cdot m^{-2} \cdot \mu m^{-1} \cdot sr^{-1}$ ]; d ~ index of agreement: 0 = no agreement, 1 = full  
 479 agreement.



480

481 Figure 6. Multi-angular differences in SIF radiance at 740 nm between a) regular, b) clumped DART  
 482 3D maize canopies and a DART simulated turbid-like canopy with LAI = 2, Spherical LAD and loamy  
 483 soil as ground. SIF radiances in the solar principal plane for the turbid-like canopy together with the  
 484 regular (RMSE = 0.42 and  $d = 0.92$ ) and the clumped (RMSE = 1.22 and  $d = 0.62$ ) maize canopies are  
 485 illustrated in c) and d), respectively (for abbreviations and symbols see Figure 5).

486 The interpretation of canopy architectural effects can be taken further by investigating the  
 487 multi-angular differences for  $SIF_{TOC}$  at 686 (Figure 5) and 740 nm (Figure 6), computed  
 488 between the turbid-like vegetation canopy, i.e., a random distribution of many small leaf facets  
 489 with the Spherical LAD, and the maize regular and clumped canopies of much larger leaves,  
 490 both with LAI = 2. DART simulated multi-angular  $SIF_{TOC}$  values of the turbid-like and regular  
 491 maize canopies at 686 nm are very close (RMSE = 0.27  $W.m^{-2}.\mu m^{-1}.sr^{-1}$ ,  $d = 0.9$ ) (see Figure

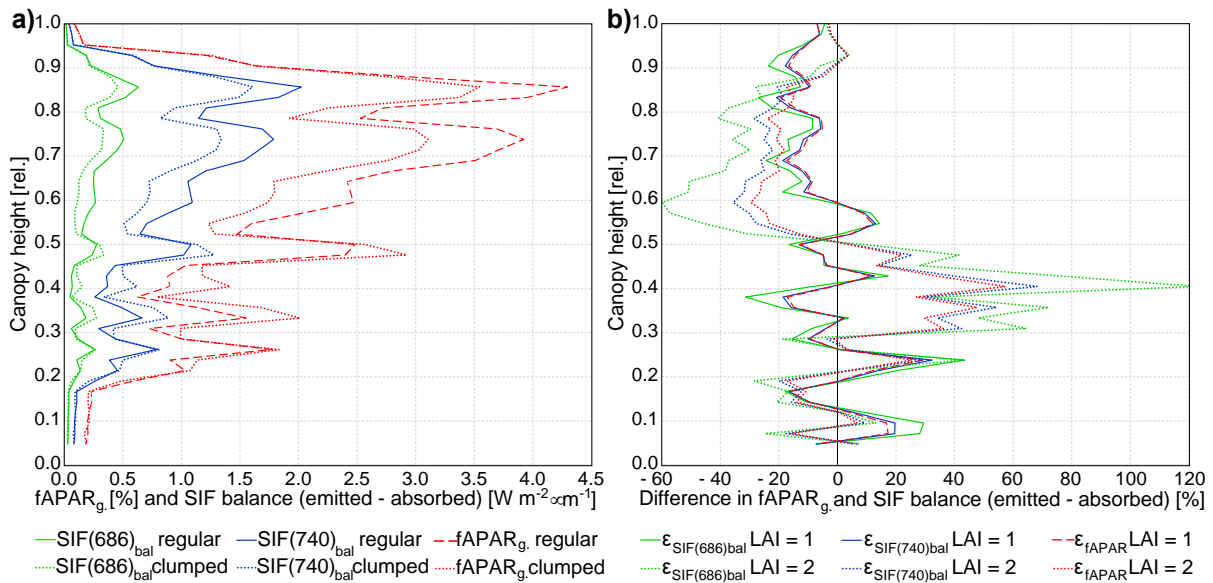
## 2.1 VEGETATION SIMULATED AS FACETS

492 5ac), indicating rather similar SIF absorptions within canopies and by soil. The maximum  
493 difference of just about  $-0.4 \text{ W.m}^{-2}.\mu\text{m}^{-1}.\text{sr}^{-1}$  appeared in very oblique viewing directions, in  
494 which maize plants scattered less SIF. Despite its slightly lower  $f\text{APAR}_{\text{green}}$  (0.68 vs. 0.72), the  
495 maize canopy scattered a bit more SIF in viewing directions around nadir and hotspot,  
496 producing a positive difference. This is caused by the maize geometrically explicit non-random  
497 LAD and large-sized leaf facets, redirecting the scattered SIF prevalingly in these directions.  
498 Larger size of maize leaves is decreasing scattering of photons, and consequently the diffuse  
499 fluxes, and causing a broader base of the  $\text{SIF}_{\text{TOC}}$  hotspot peak, observed when comparing the  
500 hotspots regions of maize and the turbid-like medium simulations. Although the multi-angular  
501 pattern for the clumped maize canopy looks also very similar ( $\text{RMSE} = 0.36 \text{ W.m}^{-2}.\mu\text{m}^{-1}.\text{sr}^{-1}$ ,  $d$   
502  $= 0.81$ ), the differences are all negative and significantly larger, with the maximum of about -  
503  $0.75 \text{ W.m}^{-2}.\mu\text{m}^{-1}.\text{sr}^{-1}$  (Figure 5bd). It means that the 50% foliage clumping increased scattering  
504 and the subsequent within-canopy absorption of SIF at 686 nm, because SIF absorption by the  
505 loamy soil beneath the clumped canopy was 7% lower than in the regular canopy, i.e., unable  
506 to cause the  $\text{SIF}_{\text{TOC}}$  reduction. The angular distributions of the same differences at 740 nm look  
507 different (Figure 6), as they are ruled mainly by scattering related to the canopy architecture.  
508 The decrease in intensity of maize far-red  $\text{SIF}_{\text{TOC}}$  is driven by the species-specific foliage  
509 distribution and geometry, significantly larger maize leaf size combined with a high leaf single  
510 scattering albedo at 740 nm and the soil absorption.  $\text{SIF}_{\text{TOC}}$  differences in Figure 6 are negative  
511 for both regular ( $\text{RMSE} = 0.42 \text{ W.m}^{-2}.\mu\text{m}^{-1}.\text{sr}^{-1}$ ,  $d = 0.92$ ) and clumped canopy of  $\text{LAI} = 2$ , but  
512 larger for the latter one ( $\text{RMSE} = 1.22 \text{ W.m}^{-2}.\mu\text{m}^{-1}.\text{sr}^{-1}$ ,  $d = 0.62$ ). Results of DART radiative  
513 budget revealed that the introduction of clumping did not increase but lowered (by 12%) the  
514 amount of soil intercepted and absorbed SIF. Hence, it is not soil but clumping-induced within  
515 canopy SIF optical interactions that are responsible for this extra reduction of  $\text{SIF}_{\text{TOC}}$ .

516 The relative contribution from different canopy parts (horizontal layers) to  $\text{SIF}_{\text{TOC}}$  and its  
517 modulation by  $f\text{APAR}_{\text{green}}$  or by SIF scattering and absorption can be investigated by plotting  
518 vertical canopy height profiles of  $f\text{APAR}_{\text{green}}$  together with corresponding SIF balances of both  
519 fluorescence wavelengths. Figure 7a shows that SIF balances are positive at all heights, i.e.,  
520 every layer act as a SIF source, and they follow, in general, changes in  $f\text{APAR}_{\text{green}}$ . The foliage  
521 clumping decreased significantly  $f\text{APAR}_{\text{green}}$ ,  $\text{SIF}(\lambda)_{\text{bal}}$  and also  $\text{SIF}_{\text{omni}}(\lambda)_{\text{esc}}$  (not shown) in  
522 the upper half of the canopy with  $\text{LAI} = 2$ , causing the overall reduction of  $\text{SIF}_{\text{TOC}}$ , but it



523 increased all of them in canopy parts below. It means that the lower leaves of the clumped  
 524 canopy contributed to the simulated  $SIF_{TOC}$  more than the same leaves of the regular canopy.



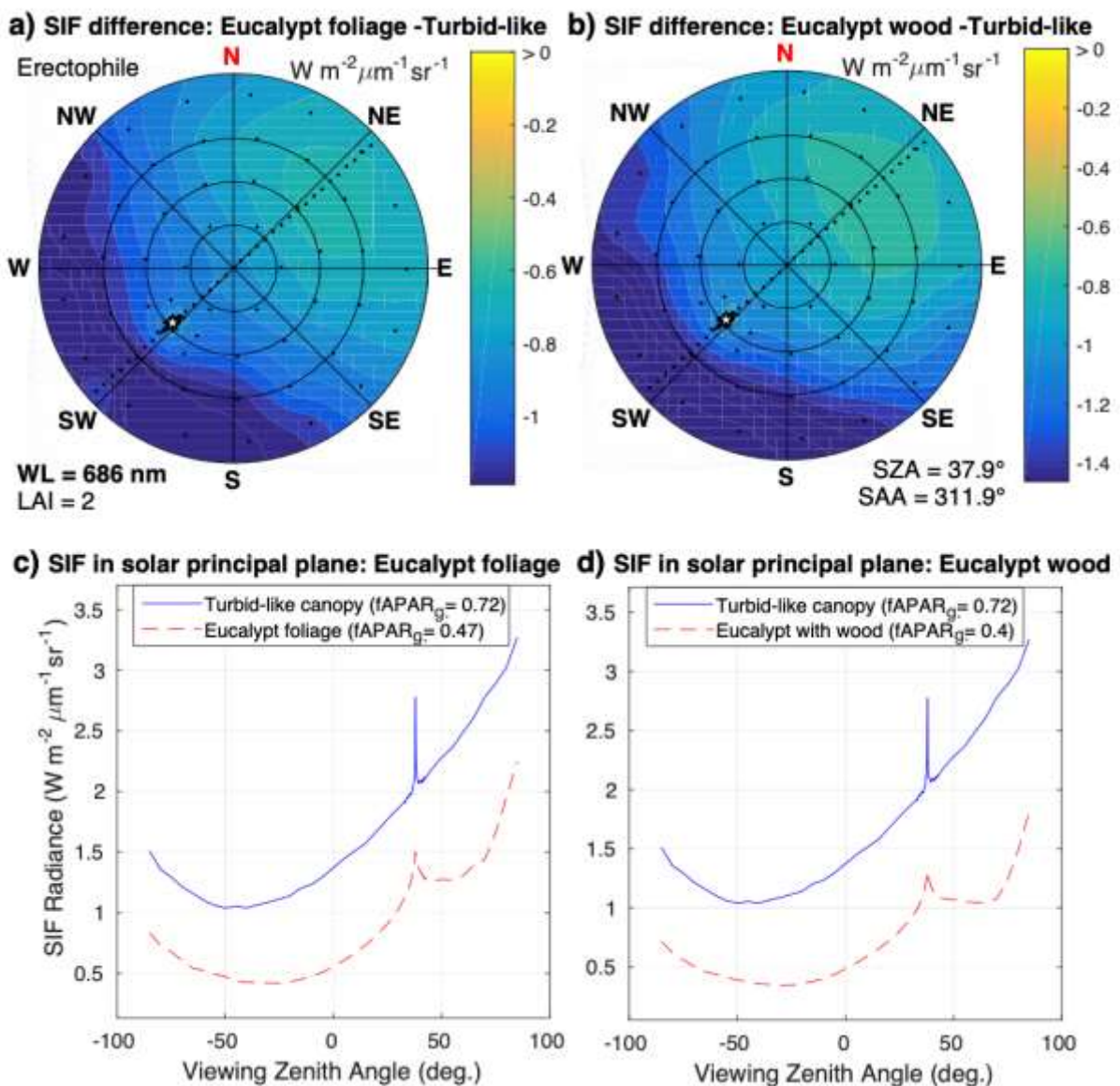
525  
 526 Figure 7. Vertical profiles of a)  $fAPAR_{green}$ , SIF balances (for maize canopies of LAI = 2) and b)  
 527 their relative differences at 686 and 740 nm computed between regularly spaced and clumped  
 528 canopies of the same LAI (for LAI = 1 and 2). Each 2.5 cm thick canopy layer is presented as a  
 529 point of the relative canopy height [0-1]. For details about computations of  $fAPAR_{green}$ , SIF  
 530 balance ( $SIF(\lambda)_{bal}$ ) and their relative differences ( $\epsilon_{fAPAR(\lambda)}$  and  $\epsilon_{SIF(\lambda)_{bal}}$ ) see section 2.4.

531 Figure 7b, depicting the  $fAPAR_{green}$  and  $SIF(\lambda)_{bal}$  relative differences between the regular  
 532 and clumped canopies, provides a further insight in this behaviour and dependencies between  
 533 SIF and  $fAPAR_{green}$  radiative budgets. It illustrates a clumping-induced steady reduction of  
 534  $fAPAR_{green}$  and SIF balance differences in upper 40% of the canopy with LAI = 1, whereas the  
 535 differences in lower 60% fluctuate between positive and negative values.  $\epsilon_{SIF(740)_{bal}}$  for  
 536 LAI = 1 follows quite closely  $\epsilon_{fAPAR(\lambda)}$ , suggesting that variability of SIF fluxes at 740 nm is  
 537 ruled mainly by clumping-induced changes in distribution of shadows and sun flecks, while  
 538  $\epsilon_{SIF(686)_{bal}}$  shows a bit more negative or positive deviations from  $\epsilon_{fAPAR(\lambda)}$ , caused by a local  
 539 increase or decrease in chlorophyll absorption of SIF at 686 nm.  $SIF_{TOC}$  for LAI = 2 is formed  
 540 by steady but greater negative differences in the canopy top half that are partially balanced out  
 541 by nearly 2-fold larger positive differences between 30 and 50% of the canopy relative height.  
 542 Comparable differences for both LAI cases between the bottom and 30% of the canopy height  
 543 indicate very similar  $fAPAR_{green}$  and SIF radiative budgets, driven by mostly diffused low-  
 544 intensity PAR. The negative  $\epsilon_{fAPAR(\lambda)}$  and  $\epsilon_{SIF(\lambda)_{bal}}$  values in the upper half of the canopy are

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545 caused by combination of higher (doubled) LAI with foliage clumping that increased internal  
 546 shadowing and consequently reduced  $fAPAR_{green}$ . It also enhanced a number of SIF photons  
 547 interacting with leaf facets, resulting in a higher fluorescence absorption, especially at 686 nm.  
 548 Scientifically interesting is the opposite behaviour between 30 and 50% of the canopy height,  
 549 where it boosted  $fAPAR_{green}$  and consequently SIF emissions, but simultaneously diminished  
 550 SIF absorption, which is evidenced by  $\epsilon_{SIF(686)_{bal}}$  and  $\epsilon_{SIF(740)_{bal}} > \epsilon_{fAPAR(\lambda)}$ . The total energy  
 551 released from these positive  $SIF(\lambda)_{bal}$  differences was, nevertheless, unable to fully compensate  
 552 the negative  $SIF(\lambda)_{bal}$  differences induced by clumping in the upper canopy parts (Figure 7a).

### 553 3.5 Impacts of foliage clumping and wood of white peppermint trees



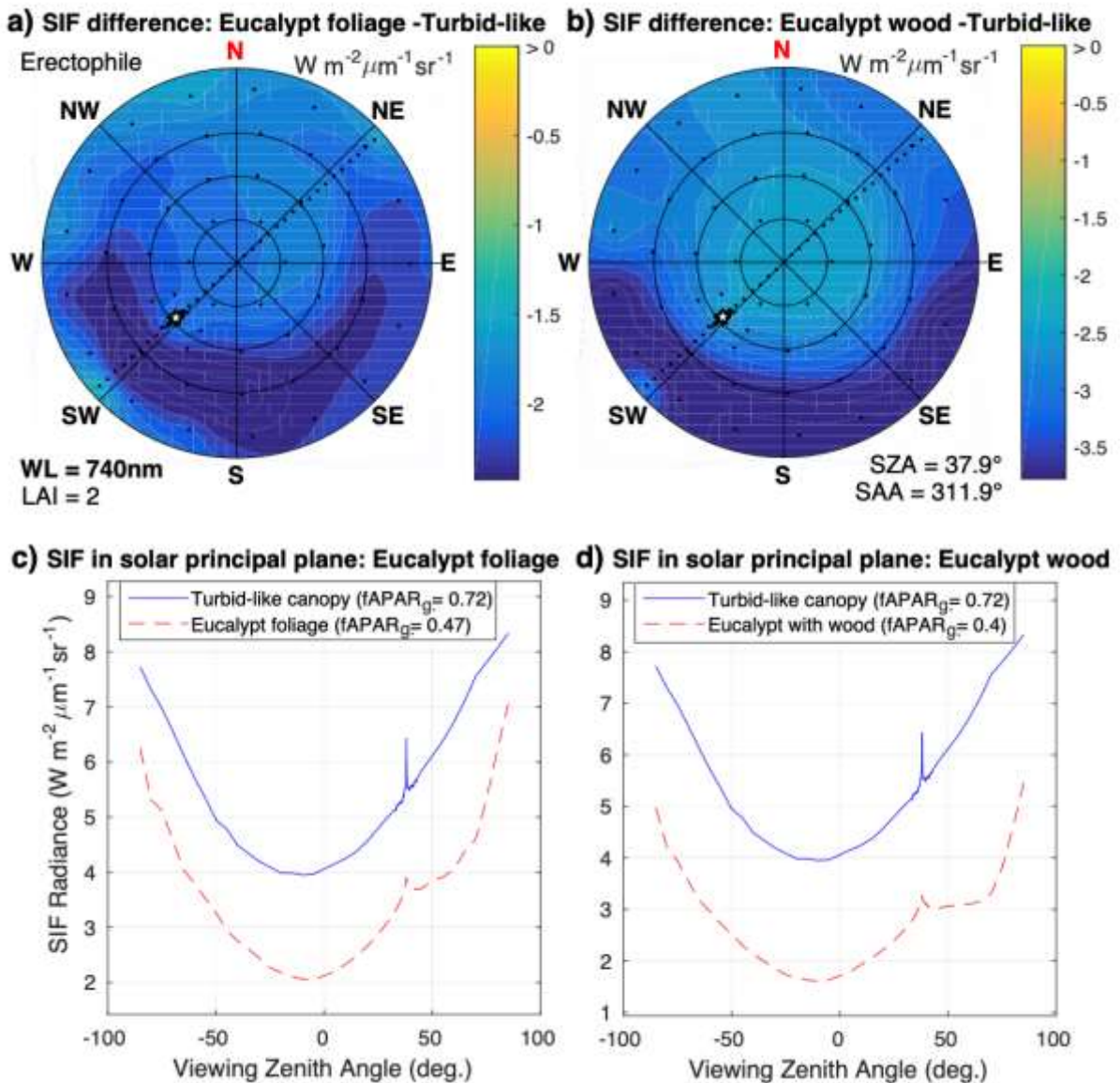
554



555 Figure 8. Multi-angular differences in SIF radiance at 686 nm between a) a dense eucalyptus canopy  
556 created only by foliage, b) the same canopy containing also woody components and a DART simulated  
557 turbid-like canopy, all with LAI = 2, Erectophile LAD and loamy soil as ground. SIF radiances in the  
558 solar principal plane for the turbid-like canopy together with the foliage-only (RMSE = 0.82 and  $d =$   
559 0.55) and the foliage with wood (RMSE = 1.0 and  $d = 0.47$ ) eucalypt canopies are illustrated in c) and  
560 d), respectively (for abbreviations and symbols see Figure 5).

561 DART 3D modelling allowed us to investigate previously unquantified impacts of foliage  
562 structure and woody material on  $fAPAR_{green}$  and on optical interactions of SIF photons inside  
563 white peppermint canopies. Figure 3 shows nadir PSII SIF<sub>TOC</sub> images at 740 nm for dense  
564 eucalyptus forest canopies without and with presence of the woody parts. A simple visual  
565 comparison of the two images reveals a lower SIF<sub>TOC</sub> in the lower right corner of the image  
566 caused by a deeper shadowing after inclusion of trunks and branches. One can also detect  
567 several large non-fluorescing branches in the SIF<sub>TOC</sub> image, visible due to a strong reflection  
568 of far-red SIF photons by peppermint bark ( $\rho_{740\text{ nm}} \approx 50\%$ ).

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569

570 Figure 9. Multi-angular differences in SIF radiance at 740 nm between a) a dense eucalyptus canopy  
 571 created only by foliage, b) the same canopy containing also woody components and a DART simulated  
 572 turbid-like canopy, all with LAI = 2, Erectophile LAD and loamy soil as ground. SIF radiances in the  
 573 solar principal plane for the turbid-like canopy together with the foliage-only (RMSE = 1.93 and d =  
 574 0.47) and the foliage with wood (RMSE = 2.68 and d = 0.35) eucalypt canopies are illustrated in c) and  
 575 d), respectively (for abbreviations and symbols see Figure 5).

576 In comparison with the multi-directional SIF radiance of the turbid-like canopy, the dense  
 577 eucalyptus stand without wood showed statistically significant decreases in  $SIF_{TOC}$  at 686 nm  
 578 (RMSE =  $0.82 W \cdot m^{-2} \cdot \mu m^{-1} \cdot sr^{-1}$ ,  $d = 0.55$ ) (Figure 8ac) and even greater at 740 nm (RMSE =  
 579  $1.93 W \cdot m^{-2} \cdot \mu m^{-1} \cdot sr^{-1}$ ,  $d = 0.47$ ) (Figure 9ac). This drop, reaching up to  $-1.2 W \cdot m^{-2} \cdot \mu m^{-1} \cdot sr^{-1}$  and  
 580 almost  $-2.5 W \cdot m^{-2} \cdot \mu m^{-1} \cdot sr^{-1}$ , respectively, can be explained by the Erectophile LAD of the  
 581 small-sized narrow white peppermint leaves, and by their strong and spatially irregular

582 clumping at the branch level. Presence of woody structures did not change considerably the  
 583 angular patterns of the SIF<sub>TOC</sub> differences, but caused its further suppression at 686 nm (RMSE  
 584 = 1.0 W.m<sup>-2</sup>. μm<sup>-1</sup>.sr<sup>-1</sup>, d = 0.47) (Figure 8bd) and even larger differences at 740 nm (RMSE =  
 585 2.68 W.m<sup>-2</sup>. μm<sup>-1</sup>.sr<sup>-1</sup>, d = 0.35) (Figure 9bd). Interestingly, it deepened the shape the solar  
 586 principal plane SIF<sub>TOC</sub> curve in back-scattering oblique viewing directions behind the hotspot  
 587 region, producing the maximum difference of almost -1.4 W.m<sup>-2</sup>. μm<sup>-1</sup>.sr<sup>-1</sup> at 686 nm and  
 588 around -3.7 W.m<sup>-2</sup>. μm<sup>-1</sup>.sr<sup>-1</sup> at 740 nm.

589 The DART ability to simulate forest stands with and without woody elements opened an  
 590 opportunity for quantification of their potential impacts on SIF emitted, observed and escaped  
 591 in the nadir direction from white peppermint dense and sparse canopies (Table 2). We  
 592 quantified the wood shading effect, causing changes in canopy fAPAR<sub>green</sub> due to the scattering  
 593 and absorption of iPAR, and the obstruction (blocking) effect of eucalyptus wood, caused by  
 594 scattering and absorption of SIF photons by bark. As expected, wood shadowing lowered SIF  
 595 emitted at both investigated wavelengths by the percentage equal to the fAPAR<sub>green</sub> reduction,  
 596 i.e., by 17.0% for the dense and 9.7% for the sparse canopy. Comparison of the foliage only  
 597 SIF<sub>TOC</sub> with the foliage and wood SIF<sub>TOC</sub> revealed lesser impacts at 686 nm than at 740 nm.  
 598 SIF escape probability factors of the simulated eucalyptus canopies were generally low:  
 599 SIF<sub>nadir(686)</sub><sub>esc</sub> ≤ 0.15 and SIF<sub>nadir(740)</sub><sub>esc</sub> ≤ 0.27. Overall, the wood obstruction effect was  
 600 greater on far-red than red SIF escape factors, causing a consistent decrease of 4-6% in  
 601 SIF<sub>nadir(740)</sub><sub>esc</sub>, but almost no change in SIF<sub>nadir(686)</sub><sub>esc</sub> for the sparse and less than 2%  
 602 increase for the dense canopy (Table 2).

603

604 Table 2. DART simulated impacts of woody material and bark on fAPAR<sub>green</sub> of leaves, SIF leaf  
 605 emissions, nadir top-of-canopy SIF<sub>TOC</sub> and nadir SIF escape probability factor at 686 and 740 nm of two  
 606 white peppermint (*Eucalyptus pulchella*) stands with dense and sparse canopy covers (CC) and LAI =  
 607 2.5. The relative impact on canopy SIF emitted by leaves (Bold fonts), is caused either by shadows  
 608 casted on photosynthetically active foliage (*shading effect*; Eq. 8) or by absorption and scattering of SIF  
 609 photons by bark-covered wood in combination with green foliage (*obstruction effect*; Eq. 11); (↓)  
 610 indicates a decreasing and (↑) an increasing effect.

DART scenario	Dense canopy (CC ≈ 80%)			Sparse canopy (CC ≈ 40%)		
	Foliage only	Foliage & Wood	<b>Relative impact [%]</b>	Foliage only	Foliage & Wood	<b>Relative impact [%]</b>
fAPAR <sub>green</sub> of leaves	0.466	0.399		0.306	0.279	

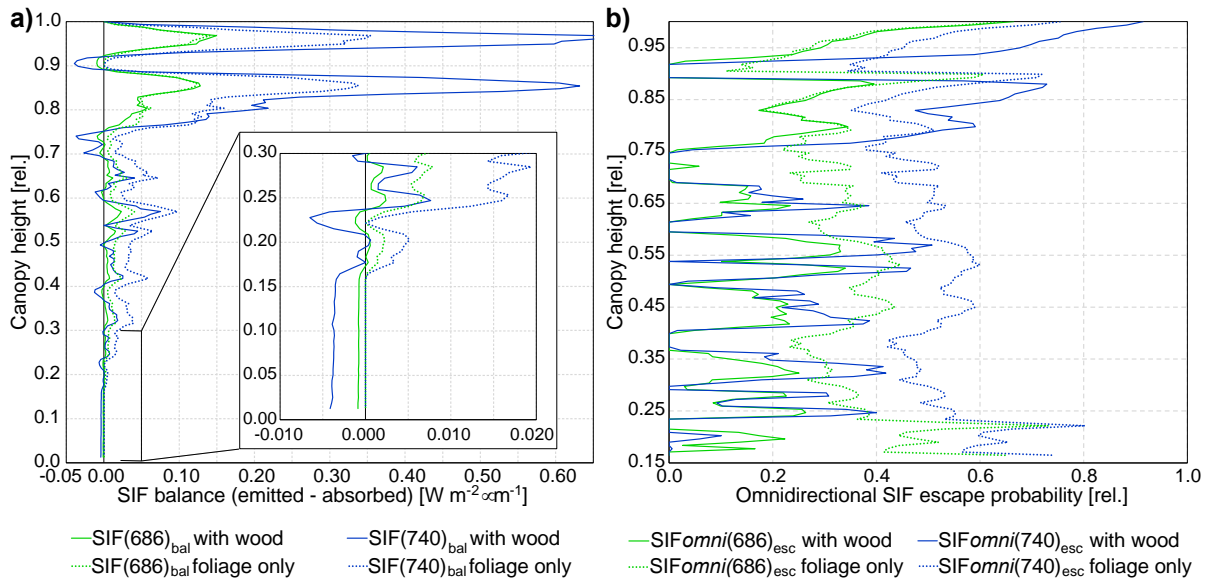
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<i>Shading effect</i> ( $\epsilon_{fAPAR(400-750)}$ )			<b>17.0</b> (↓)		<b>9.7</b> (↓)	
<u>Red SIF (686 nm)</u>						
Emitted by leaves [ $W \cdot m^{-2} \cdot \mu m^{-1}$ ]	11.626	9.939	7.618	6.945		
Nadir $SIF_{TOC}$ [ $W \cdot m^{-2} \cdot \mu m^{-1} \cdot sr^{-1}$ ]	0.554	0.481	0.303	0.275		
$SIF_{nadir(686)_{esc}}$ [rel.]	0.150	0.152	0.125	0.124		
<i>Obstruction effect</i> ( $\epsilon_{SIF(686)_{esc}}$ )			<b>-1.5</b> (↑)		<b>0.6</b> (↓)	
<u>Far-red SIF (740 nm)</u>						
Emitted by leaves [ $W \cdot m^{-2} \cdot \mu m^{-1}$ ]	24.461	20.914	16.029	14.613		
Nadir $SIF_{TOC}$ [ $W \cdot m^{-2} \cdot \mu m^{-1} \cdot sr^{-1}$ ]	2.093	1.693	1.260	1.108		
$SIF_{nadir(740)_{esc}}$ [rel.]	0.269	0.254	0.247	0.238		
<i>Obstruction effect</i> ( $\epsilon_{SIF(740)_{esc}}$ )			<b>5.7</b> (↓)		<b>3.6</b> (↓)	

611

612 More detailed understanding of the wood-induced effects inside the dense white  
613 peppermint canopy can be obtained from analysing its DART-simulated vertical profiles of SIF  
614 balances and omnidirectional SIF escape factors. Plots of  $SIF(\lambda)_{bal}$  in Figure 10a and  
615  $SIF_{omni}(\lambda)_{esc}$  in Figure 10b, shown across the relative stand height, revealed two significant  
616 findings. First, every leaf-containing part of the canopy comprised of only foliage is acting as  
617 a SIF source ( $SIF_{omni}(\lambda)_{esc} > 0$ ), but the presence of woody components turned the parts  
618 emitting only a little fluorescence into SIF sinks ( $SIF_{omni}(\lambda)_{esc} = 0$ ). Second, a majority of the  
619  $SIF_{TOC}$  signal originates from leaves occupying top 25% percent of the eucalyptus canopy  
620 height. Although the close-up of the 0-30% canopy height section in Figure 10a shows a strong  
621 SIF absorption by trunks and lower branches that results in  $SIF(\lambda)_{bal} < 0$  (especially at 740 nm),  
622 different SIF energy budget results were obtained for top 25% (i.e., 75-100%) of the canopy.  
623 The wood presence in this highly emitting canopy part increased the  $SIF(686)_{bal}$  values only  
624 negligibly, as the bark and photosynthesizing leaves were capable of absorbing nearly all extra  
625 SIF photons reflected at 686 nm by woody structures. This result is in line with a very slight  
626 increase of  $SIF_{nadir(686)_{esc}}$  listed in Table 2. Wood presence, however, decreased absorptance  
627 and increased more than 2-fold reflectance of SIF at 740 nm, which significantly enhanced  
628 (almost doubled) the  $SIF(740)_{bal}$  values in this upper canopy part. Despite this limited local  
629 boost, wood obstructions suppressed values of both  $SIF(740)_{bal}$  and  $SIF_{omni}(740)_{esc}$  in the rest

630 of the canopy profile, leading to an overall 5.7% reduction in canopy  $SIF_{nadir}(740)_{esc}$   
 631 (Table 2) and, consequently, in a decrease of multi-angular  $SIF_{TOC}$  (Figure 9ab).



633 Figure 10. Vertical profiles of a) SIF balances ( $SIF(\lambda)_{bal}$ ) and b) relative omnidirectional SIF  
 634 escape factors ( $SIF_{omni}(\lambda)_{esc}$ ) at 686 and 740 nm for a dense white peppermint (*Eucalyptus*  
 635 *pulchella*) canopy ( $CC \approx 80\%$  and  $LAI = 2$ ) created only by foliage (dashed lines) and the same  
 636 canopy containing also woody components (solid lines). Each 10 cm thick canopy layer is  
 637 presented as a point of the relative canopy height [0-1]. For details about computations of  $SIF(\lambda)_{bal}$   
 638 and  $SIF_{omni}(\lambda)_{esc}$  see section 2.4.

640 **4. Discussion**

641 **4.1 Comparison of DART and SCOPE/mSCOPE models**

642 DART outputs were nearly in a perfect agreement with the corresponding results obtained  
 643 for simple, turbid medium vegetation scenes with SCOPE and mSCOPE. Better agreements  
 644 were obtained for the  $SIF_{TOC}$  local maximum at 686 nm, where the signal is attenuated by the  
 645 SIF chlorophyll absorption. Since the  $SIF_{TOC}$  values at 740 nm are controlled dominantly by  
 646 canopy structural traits, the smallest discrepancies were obtained for the geometrically more  
 647 uniform Planophile LAD. Here, the  $SIF_{TOC}$  signal is dominated by the first order scattering of  
 648 prevalingly horizontally oriented leaves, lowering the occurrence of fluorescence absorption.  
 649 The largest multi-angular  $SIF_{TOC}$  differences in all tested LAD and LAI scenarios occurred in  
 650 very oblique viewing angles, in which the modelled radiance is impacted by uncertainties in  
 651 angular discretization of the upper hemisphere.

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652 Despite of a generally high agreement with SCOPE/mSCOPE simulations, this model cross  
653 comparison is not a fully sufficient replacement of an independent validation of the DART  
654 model, which is expected to be performed with real canopy SIF<sub>TOC</sub> measurements in a near  
655 future. Nonetheless, this comparison provides the evidence that current integration of the  
656 Fluspect model and implementation of the 3D flux-tracking radiative transfer of SIF emitted  
657 from geometrically explicit leaves are as plausible as already validated 1D radiative transfer  
658 modelling approaches of SCOPE and mSCOPE models (Migliavacca et al. 2017; Pacheco-  
659 Labrador et al. 2019; van der Tol et al. 2016; Vilfan et al. 2019). This conclusion provides us  
660 with a high level of confidence that the radiative transfer modelling of SIF in DART can be  
661 used to investigate the major canopy structural controls of SIF<sub>TOC</sub> in geometrically explicit 3D  
662 canopies, which structural complexity cannot be represented and tested in SCOPE or mSCOPE.

### 663 **4.2 SIF changes due to classification of sun-/shade-adapted leaves and canopy structure**

664 Distinct parametrization of sun- and shade-adapted leaves did not result in major  
665 differences in SIF<sub>TOC</sub>, but other canopy structural parameters were found to be more important.  
666 The specific distinction of leaf *fqe* for sun- and shade-adapted foliage appeared to have a smaller  
667 impact on DART simulated nadir SIF<sub>TOC</sub> than increasing LAI and foliage clumping reducing  
668 CC from 100% to 50% (c.f., Figure 1 and Figure 3). Yet, the impact of the leaf-light adaptation  
669 effect might increase, if a DART user applies Q double-threshold values that favour strongly  
670 the shade- over the sun-adapted class and simultaneously increases the PSI and PSII *fqe* inputs.  
671 Secondly, the influence of the shade-adapted class would be more significant when tested for  
672 naturally more clumped and taller (e.g., forest) canopies. Therefore, identification of correct Q  
673 thresholds and sun/shade *fqe* values are, together with measurements of canopy gaps and foliage  
674 clumping, essential for further investigation of the photosynthetic light adaptations and their  
675 impacts on SIF<sub>TOC</sub>.

676 When evaluating impacts of maize canopy structural traits, our nadir SIF<sub>TOC</sub> results  
677 indicated a general superior role of LAI over the foliage clumping. However, doubling the  
678 foliage clumping of maize crop with LAI = 2 caused such a strong increase in absorption of red  
679 SIF photons by chlorophylls that diminished and fully equalled the previous increase in SIF<sub>TOC</sub>  
680 between 650 and 725 nm caused by doubling the number of regularly spaced plants, i.e., twice  
681 higher LAI (Figure 2). Interpretation of DART 3D radiative budget computed for the two SIF  
682 local maximums informed us that this strong red SIF reduction took place in the upper half of

683 the canopy (specifically between 50 and 90% of the canopy height; Figure 7), because the  
684 clumping caused a slight enhancement of SIF energy fluxes in most of the lower half canopy  
685 parts and the absorption of SIF by soil background was after the clumping introduction lowered.  
686 The fact that relative differences of red SIF balances in upper halves of the clumped and  
687 unclumped canopies are 2-fold more negative than the same differences of  $fAPAR_{green}$  (Figure  
688 7b) indicates that the increase in foliage shadowing is responsible only for a half of this  
689 clumping-induced SIF reduction. The second half is caused by a more frequent recollision and  
690 consequent greater absorption of red SIF photons by leaf photosynthetic pigments. Clumping  
691 driven results for  $LAI = 1$  showed less consistent and milder effects, which means that canopy  
692 must have a certain minimal leaf density to produce these interactions.

693 Clumping impacts caused by decreasing CC can be also demonstrated on the example of  
694 white peppermint stands without woody material. According to results listed in Table 2,  
695 decrease of CC from 80% to 40% triggered a reduction in  $fAPAR_{green}$  and, consequently, in  
696 emitted SIF by 34%, and simultaneously lowered the  $SIF_{TOC}$  by 45% at 686 nm and by 40% at  
697 740 nm. Thereby, if one accepts an assumption that scattering rates of red and far-red SIF  
698 photons by the canopy structures (including structures of a leaf interior without foliar pigments)  
699 are equal, then doubling the leaf density while keeping a constant canopy  $LAI = 2$  induced an  
700 additional 5% decrease in red  $SIF_{TOC}$  attributed to a higher red SIF absorption by chlorophylls.  
701 It is important to mention that different quantitative impacts of LAI and foliage clumping on  
702  $SIF_{TOC}$  might be revealed if the classification of sun-/shade-adapted leaves is included and  
703 different (i.e., light adaptation specific) PSI and PSII  $fqe$  values are specified by a DART user.  
704 Since the natural variability in  $fqe$  and leaf biochemistry was not accounted for in this study, a  
705 direct comparison (validation) of these results with SIF observations of real croplands or forests  
706 (e.g., Guan et al. 2015; He et al. 2020; Peng et al. 2020; Wang et al. 2020) would be misleading.

707 Multi-angular DART simulations of  $SIF_{TOC}$  demonstrate that the influence of leaf size,  
708 foliage angularity and its clumping (CC) is equally or even more crucial for modulating  $SIF_{TOC}$   
709 in oblique viewing directions. The polar plots of  $SIF_{TOC}$  at 686 nm for maize (Figure 5b) and  
710 eucalyptus (Figure 8a) canopies with  $LAI = 2$  revealed the largest influence in very oblique  
711 backward directions behind the hotspot and the smallest impact in forward directions opposite  
712 to the hotspot. The patterns of angular anisotropy for  $SIF_{TOC}$  at 740 nm are rather different. A  
713 significant impact of maize canopy structure was found around the Northern and the Southern

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714 viewing angles (Figure 6b), whereas only the Southern viewing directions were impacted by  
715 the eucalyptus canopy architecture (Figure 9a). Thus, far-red  $SIF_{TOC}$  of each architecturally  
716 distinct plant formation (i.e., plant functional type) must be approached individually and the  
717 canopy specific structural confounding effects must be removed or at least reduced before any  
718 application of remotely sensed  $SIF_{TOC}$ . This recommendation is in line with a number of recent  
719 works developing far-red  $SIF_{TOC}$  normalization approaches to mitigate the canopy structural  
720 effects (Liu et al. 2019b; Yang and van der Tol 2018; Yang et al. 2020b; Zeng et al. 2019).

### 721 *4.3 Impacts of wood structures on eucalyptus $SIF_{TOC}$ signal and $SIF$ escape factors*

722 Accounting for presence of bark-covered wood structures in our eucalyptus simulations  
723 decreased nadir 740 nm  $SIF_{TOC}$  by about 23% for the dense canopy and by 13% for the sparse  
724 canopy (Table 2). Results suggest that approximately one quarter of the total  $SIF$  reduction is  
725 caused by direct optical interactions (obstruction) of far-red  $SIF$  photons with bark surfaces in  
726 combination with green leaves under the natural geometrical distributions, whereas three  
727 quarters of the reduction resulted from the reduction in  $APAR_{green}$  due to wood shadowing.  
728 Having the bark reflectance and absorptance at 740 nm both equal to 50%, the wood structures  
729 of white peppermint trees acted, on one hand, as strong reflectors and boosted the far-red  $SIF$   
730 emission produced in top 25% of the dense canopy (Figure 10a). On the other hand, they acted  
731 as a far-red  $SIF$  sink in the rest of the canopy, i.e., in lower 75% of the canopy relative height.  
732 Although it is expected that tree species with a lower bark near infrared reflectance will  
733 demonstrate radiative budgets with a higher far-red  $SIF$  obstruction (absorptance), the  
734 consistently decreasing nadir obstruction effects of both modelled eucalyptus stand indicate that  
735 the wood obstruction is a regular confounding factor that must be treated as a systematic error  
736 source. Therefore, it should be accounted for, or if feasible even corrected, when interpreting  
737 far-red  $SIF_{TOC}$  data sensed remotely over forests.

738 The effect of woody material on nadir  $SIF_{TOC}$  at 686 nm was smaller, because the total pool  
739 of canopy red  $SIF$  photons originating just from PSII is naturally small and additionally reduced  
740 by absorption of photosynthetic pigments. Interestingly, the bark absorptance of 60% and  
741 reflectance of 40% at 686 nm, in combination with the specific geometry of eucalypt tree  
742 crowns (i.e., a strong branch foliage clumping with Erectophile LAD), decreased the red  $SIF$   
743 nadir escape factor of the sparse canopy by 0.6%, whereas the same  $SIF$  escape factor in the  
744 dense canopy was increased by 1.5%. If we accept these simulations as generally applicable,



745 we may conclude that the presence of wood affects the red SIF forest canopy balance in both  
746 negative and positive ways. However, the impact is generally small, predominantly influencing  
747 the less emitting lower 75% of the canopy height rather than larger emissions originating from  
748 top 25% of the canopy. Since we modelled and analysed only two mono-species eucalyptus  
749 stands, additional simulations for other tree species, including natural variability in species-  
750 specific optical, biochemical and structural properties, will be essential to draw more  
751 comprehensive and generic conclusions regarding the wood obstruction effects.

752 DART estimates of the relative eucalyptus canopy SIF escape factor in the nadir direction,  
753 which can be used to compute the apparent SIF efficiency (a gross primary production proxy  
754 less impacted by canopy structures; Wang et al. 2020), were quite low, smaller than 0.15 for  
755 red and 0.27 for far-red SIF. Nonetheless, the omnidirectional escape factors of individual  
756 canopy layers were higher, reaching up to 0.65 for red and 0.9 for far-red SIF in the highly  
757 emissive top 25% of the canopy height (Figure 10b). These numbers and results in Figures 9  
758 and 10 suggest that oblique multi-directional observations of forest canopies (e.g., with tower-  
759 based instruments) should capture more SIF photons than a single nadir measurement, and,  
760 thus, provide a stronger SIF<sub>TOC</sub> signal. Once again, more simulations covering different forest  
761 types and their natural variability are required to conclude if these interpretations have a general  
762 applicability or if the white peppermint canopies represent a unique and possibly extreme case..  
763 Despite a limited size of this study, we demonstrate that the entire 3D structural complexity,  
764 including woody material, must be taken into account when assessing quantity of SIF photons  
765 scattered and absorbed by canopy components and those escaping from a forest canopy.

#### 766 *4.4 Development of DART SIF modelling for large canopies and landscapes*

767 DART SIF simulations for geometrically explicit representations of terrestrial vegetation  
768 have computational limitations regarding a simulated scene size and a number of objects (i.e.,  
769 triangular facets) creating 3D mock-ups of plant canopies. Theoretically, one can create an  
770 extensive landscape occupied with an unlimited population of plants and other 3D objects (e.g.,  
771 open-water bodies, roads, buildings, etc.), but the SIF simulation, and mainly radiative budget,  
772 of such a scene might be practically unfeasible as the computer memory and processor  
773 capabilities are not unlimited. Therefore, another two approaches, allowing more efficient  
774 simulations of large canopies and extensive landscapes, are being implemented and tested in  
775 DART: i) SIF modelling for vegetation canopies represented by 3D turbid voxels (i.e., voxels

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776 filled with a vegetation turbid medium), and ii) a direct and reverse MC modelling called  
777 DART-Lux (Gastellu-Etchegorry et al. 2020). The latter one is especially highly promising for  
778 simulating extensive SIF<sub>TOC</sub> images. It uses only the landscape elements contributing to the  
779 formation of a simulated image, which decreases the computer time and memory by a factor as  
780 large as 100. Once fully tested and solidified, both approaches will provide DART users with  
781 potential satellite SIF observations adapted to common ground sampling distances of hundreds  
782 of meters. Such simulations could test multiple SIF confounding optical effects, for instance,  
783 those originating from photosynthetically inactive Earth surfaces of rough terrain  
784 configurations resulting in dynamic spatiotemporal irradiation changes and shadow patterns.

### 785 5. Conclusions

786 Physical and technical implementation of discrete anisotropic radiative transfer modelling  
787 for solar-induced chlorophyll fluorescence in geometrically explicit 3D plant canopies was  
788 described and compared with complementary cases simulated in 1D models SCOPE and  
789 mSCOPE. The cross-comparison revealed that DART simulations of SIF<sub>TOC</sub> for geometrically  
790 simple and spatially homogenous canopies produced nearly the same results as both 1D models.  
791 The largest SIF<sub>TOC</sub> differences occurred in very oblique viewing angles that are impacted by  
792 higher modelling uncertainties than the directions closer to nadir.

793 Further exploitation of DART ability to simulate SIF images and radiative budgets of  
794 virtual 3D maize crops showed that the distinction and adjustment of fluorescence efficiencies  
795 for sun- and shade-adapted leaves had a smaller impact on DART simulated SIF<sub>TOC</sub> than an  
796 increase in leaf density (LAI) and local foliage clumping. When analysing nadir SIF<sub>TOC</sub> impacts  
797 by foliar density traits, we found a superior role of LAI over the foliage clumping. Nonetheless,  
798 the foliage clumping was shown to be an important controlling factor of maize and eucalyptus  
799 SIF<sub>TOC</sub> simulated at 686 and 740 nm in oblique viewing directions, and also a crucial driver of  
800 the red SIF balance, i.e., SIF emission and absorption, in vertical profile of irregularly spaced  
801 maize crop with LAI = 2. These study outcomes must be, however, reproduced for other plant  
802 functional types to confirm and investigate further the influences of leaf light intensity  
803 adaptations and density traits on SIF variability inside and at the top of different canopies.

804 DART simulations of two white peppermint eucalyptus stands suggested that woody  
805 material has a significant impact on SIF<sub>TOC</sub>. Trunks and branches cast shadows on  
806 photosynthesizing leaves, decreasing their SIF emissions by about 15% in dense and 8% in

807 sparse canopy simulations. Although the absorbance and reflectance of eucalyptus bark (both  
808 about 50% at 740 nm), in combination with a multiple scattering and absorption by leaves,  
809 nearly doubled the pool of far-red SIF photons in the top 25% part of dense canopy, they  
810 reduced the overall canopy escape of far-red SIF in the nadir viewing direction by 6% and 4%  
811 in the sparse stand. Interestingly, the nadir escape factors of red SIF from dense and sparse  
812 canopies were almost unimpacted by presence of woody material, despite a relatively high 40%  
813 reflectance of bark at 686 nm. These unique results demonstrate that further development of  
814 SIF 3D radiative transfer modelling has a potential to reveal new insights in SIF observations  
815 of spectrally, spatially and topographically heterogeneous vegetated landscapes, acquired at  
816 different spatial scales by proximal, airborne and space-borne optical sensors.

### 817 **Acknowledgments**

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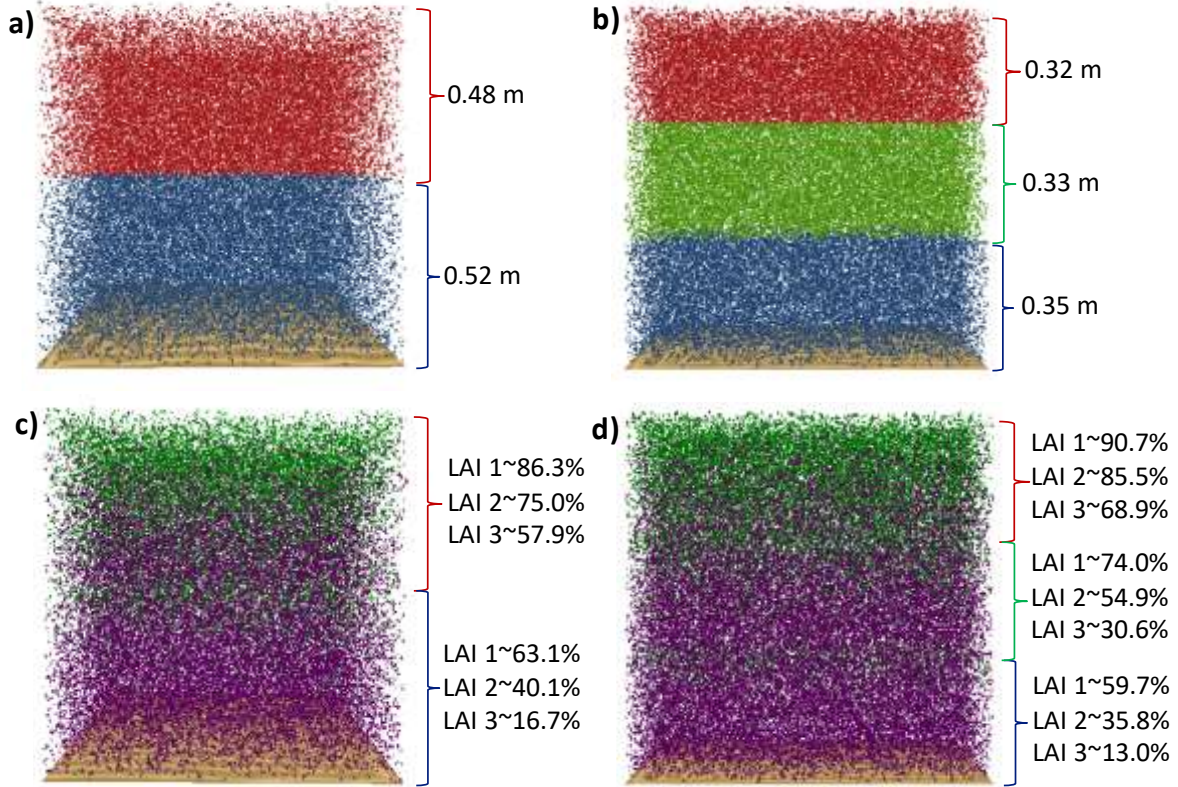
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831

832 **Appendix A: Comparison of DART and SCOPE/mSCOPE SIF radiative transfers**

833 Since SCOPE and mSCOPE are turbid medium models, we prepared DART 3D scenes  
834 mimicking their 1D canopies as closely as possible. SCOPE, mSCOPE and DART were  
835 adjusted to use the same bottom-of-atmosphere (BOA) solar direct and diffuse irradiance,  
836 simulated with DART atmosphere radiative transfer module using the United States standard  
837 atmosphere gas model (NOAA et al. 1976) and the rural area aerosol model with a visibility of  
838 23 km. The scene was a 1 m height vegetation canopy above a bare soil with three Lambertian  
839 reflectance ( $\rho$ ) properties: i) black soil ( $\rho = 0$ ), ii) half-reflective soil ( $\rho = 0.5$ ), and iii) loamy  
840 gravel brown dark soil with  $\rho$  linearly increasing with wavelength ( $\rho \approx 6\%$  at 550 nm,  $\rho \approx 12\%$   
841 at 686 nm and  $\rho \approx 15\%$  at 740 nm). Every leaf facet had the same specific Lambertian  
842 reflectance and transmittance, i.e., there was no division of leaf optical properties on sunlit or  
843 sun-adapted and shaded or shade-adapted leaves. For the DART-SCOPE comparison, the *eta*  
844 fluorescence weight parameters were forced to one. For the DART-mSCOPE comparison, we  
845 split turbid scenes into two and three almost equally high layers (see Figure A1ab). Leaves of  
846 2- and 3-layer simulations were divided into sunlit and shaded (see % of sunlit leaves in each  
847 layer in Figure A1cd) and the *eta* parameters simulated per layer for both leaf cohorts in  
848 mSCOPE were entered in the corresponding DART simulations. Leaf optical properties were  
849 simulated with the same Fluspect version, using the input parameters listed in Table A1. In  
850 attempt to simulate strong SIF<sub>TOC</sub> signals, the *fqe* values for PSI and PSII were selected close  
851 to their potential maximums. Simulations considered three leaf densities, specified by the leaf  
852 area index (LAI) equal to 1, 2 and 4. In SCOPE simulations, we tested three leaf angle  
853 distributions (LAD): Spherical, Erectophile and Planophile (Danson 1998), whereas we applied  
854 only the Spherical function, the most frequent naturally occurring LAD, in mSCOPE  
855 simulations. All leaves were homogenously distributed throughout the canopies, i.e. the foliage  
856 clumping index (Chen and Black 1992) was equal to 1. The DART leaf facets were equilateral  
857 triangles with the surface area of 0.08 cm<sup>2</sup>. Such small leaf area ensured independency of DART  
858 simulated TOC reflectance and SIF from the solar azimuth angle. The leaf width required for  
859 SCOPE/mSCOPE computations in the hot-spot direction was set to the height of DART facets,  
860 i.e., 0.37 cm. The solar azimuth angle (SAA) was fixed to 311.89° (anticlockwise from South)  
861 and the solar zenith angle (SZA) to 37.94° (i.e., solar elevation angle of 52.06°) as for  
862 Washington D.C. (USA) area (the Beltsville Agricultural Research Center; Lat. 39.03°N, Long.  
863 76.85°W) on 26<sup>th</sup> August 2014 at 14.00 local time (i.e., at 13.50 solar time). Nadir SIF<sub>TOC</sub>

864 radiance [ $\text{W}\cdot\text{m}^{-2}\cdot\mu\text{m}^{-1}\cdot\text{sr}^{-1}$ ] between 640 and 850 nm (1 nm bandwidth) was simulated for all  
 865 combinations of the input parameters with the three RTMs. The obtained PSI, PSII and total  
 866 SIF<sub>TOC</sub> values were compared statistically (as described in Section 2.6).



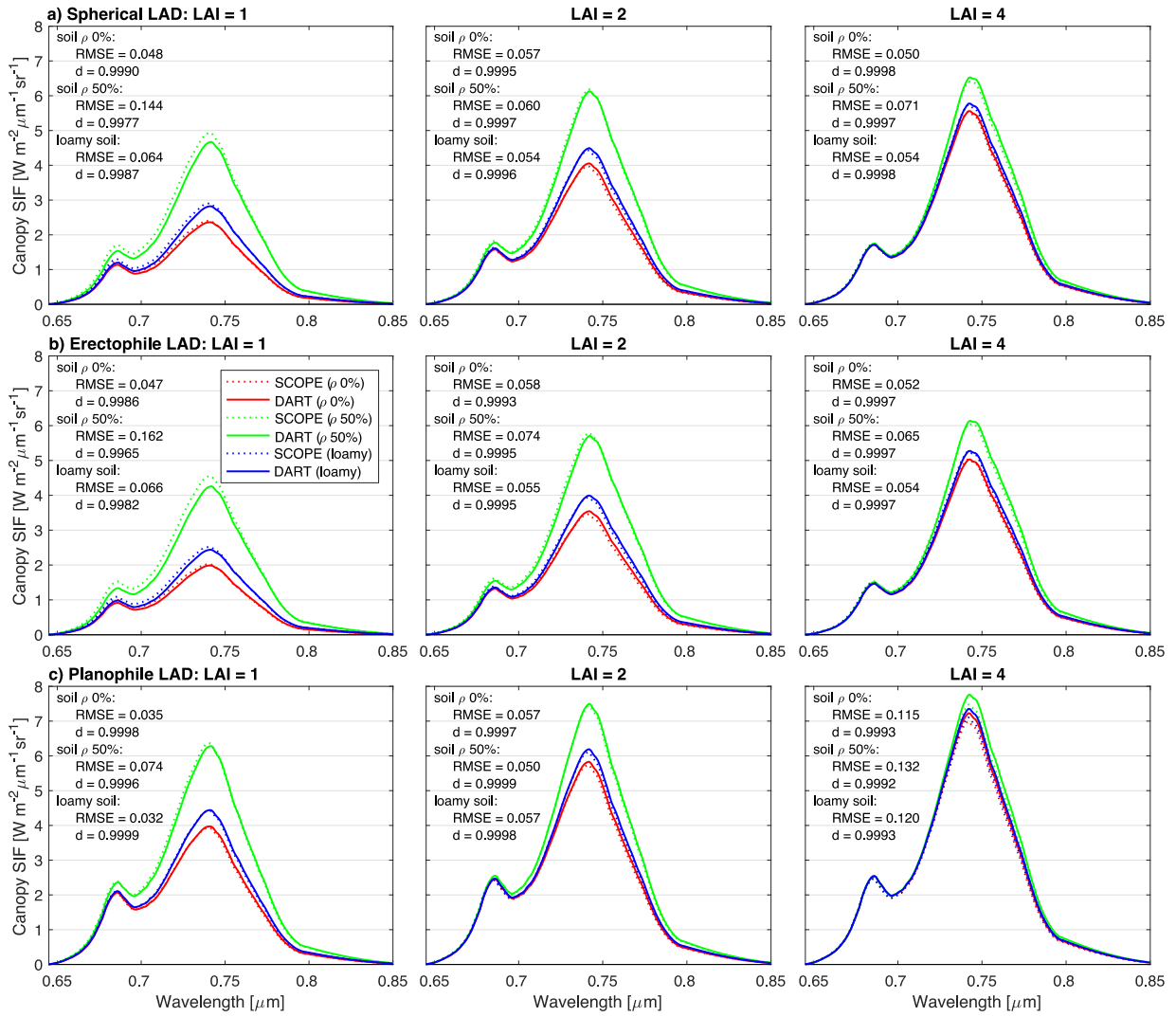
867 Figure A1. DART representations of a) 2- and b) 3-layered turbid-like canopies designed for comparison  
 868 with the mSCOPE model (numbers indicate the height of each layer). Illustration of sunlit (under direct  
 869 illumination; green) and shaded (under diffuse illumination, violet) triangular leaves for both c) 2- and  
 870 d) 3-layered canopies (numbers indicate % of sunlit leaves per layer for each simulated LAI).  
 871  
 872

873 Table A1: Input parameters of the Fluspect model used to simulate optical properties of  
 874 SCOPE/mSCOPE turbid medium leaves and corresponding DART leaves (for explanations of input  
 875 abbreviations see caption of Table 1).

Fluspect inputs	Cab	Car	EWT	LMA	N	PSI	PSII
	$[\mu\text{g}\cdot\text{cm}^{-2}]$	$[\mu\text{g}\cdot\text{cm}^{-2}]$	[cm]	$[\text{g}\cdot\text{cm}^{-2}]$		<i>fqe</i>	<i>fqe</i>
(m)SCOPE layers							
mSCOPE first layer (from top)	40	10	0.006	0.0014	1.0	0.006	0.03
SCOPE & mSCOPE second layer	60	15	0.009	0.0021	1.5	0.006	0.03
mSCOPE third layer (from top)	80	20	0.012	0.0028	2	0.006	0.03

876

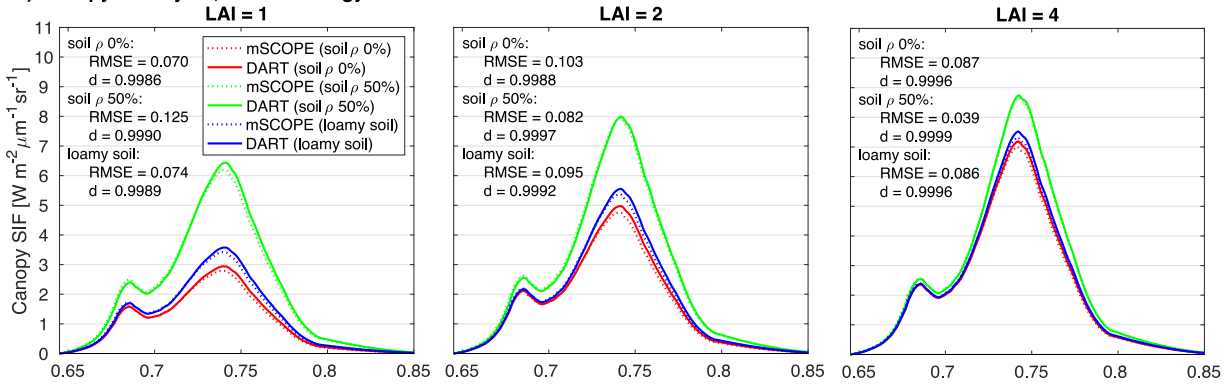
## 2.1 VEGETATION SIMULATED AS FACETS



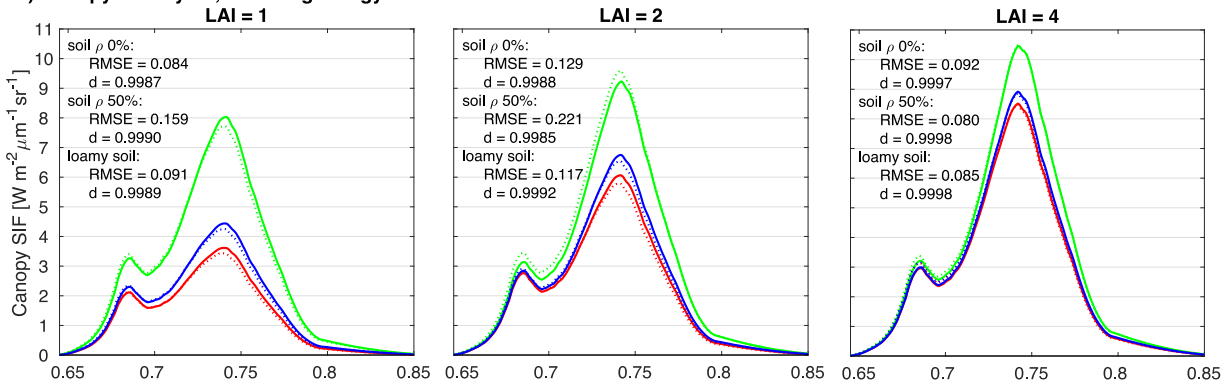
877

878 Figure A2. DART and SCOPE total nadir SIF of vegetation canopies with LAI=1, 2 and 4, three soils ( $\rho$   
 879 = 0%,  $\rho = 50\%$ ,  $\rho =$  loamy dark gravel soil), and with a) Spherical, b) Erectophile, and c) Planophile  
 880 LAD (RMSE ~ root mean square error; d ~ index of agreement: 0 = no agreement, 1 = full agreement).

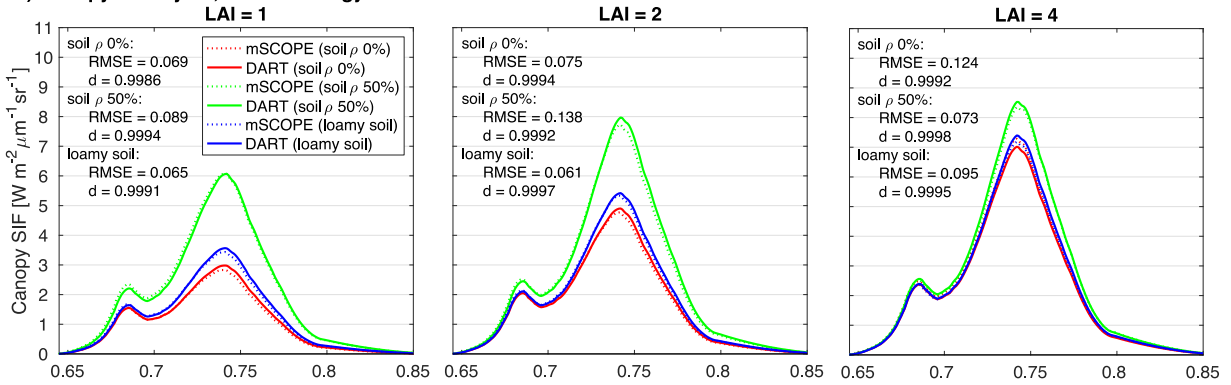
a) Canopy of 2 layers, without energy balance:



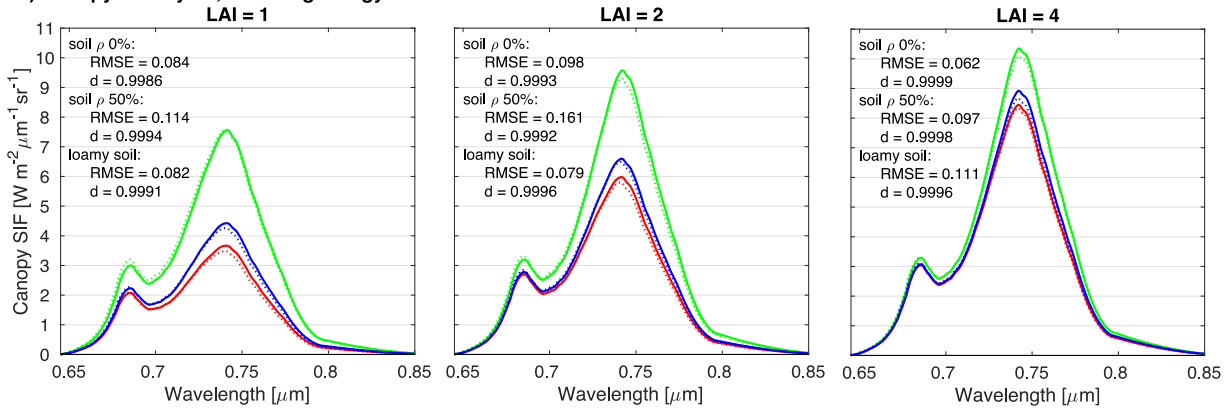
b) Canopy of 2 layers, including energy balance:



c) Canopy of 3 layers, without energy balance:



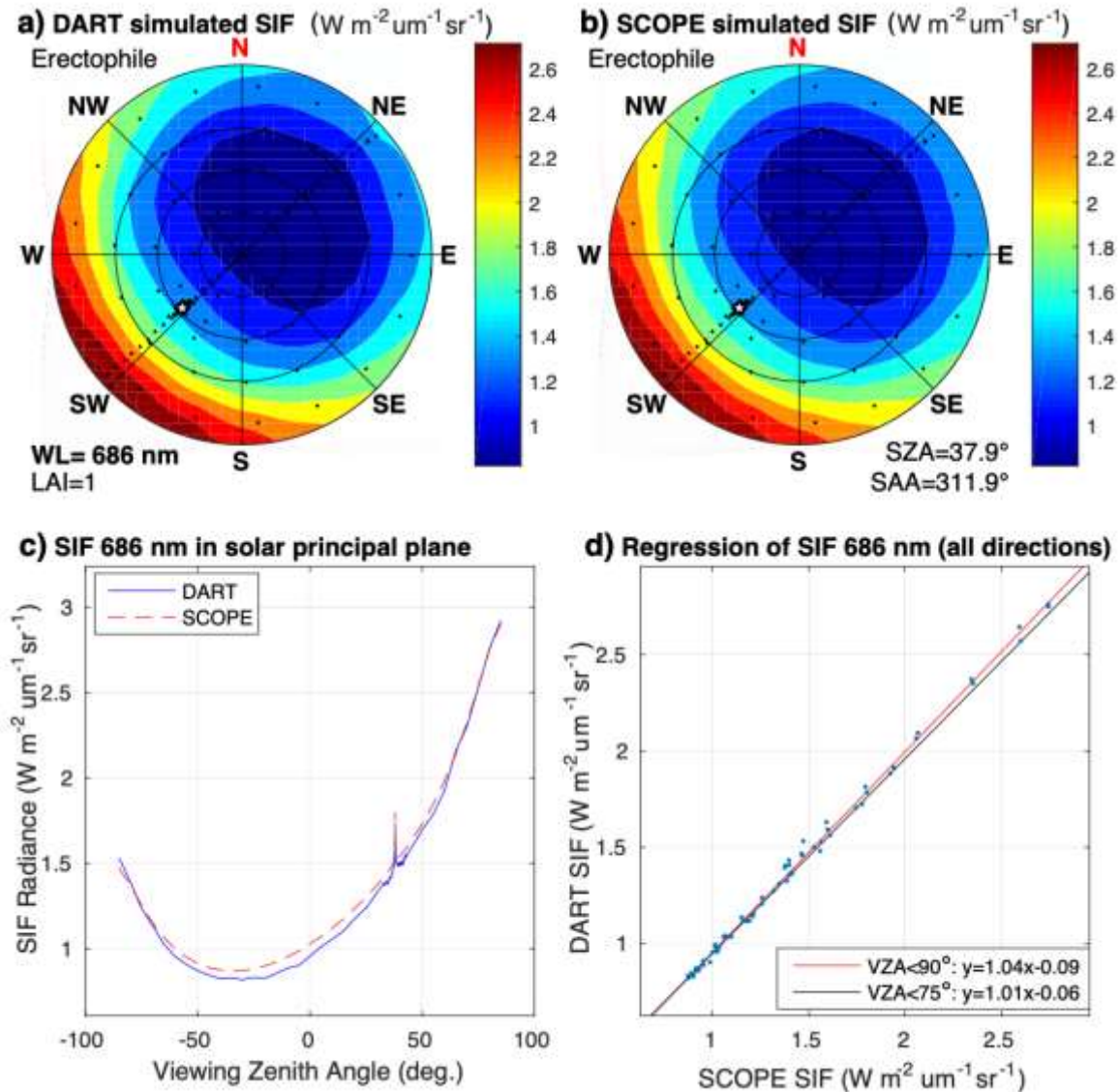
d) Canopy of 3 layers, including energy balance:





## 2.1 VEGETATION SIMULATED AS FACETS

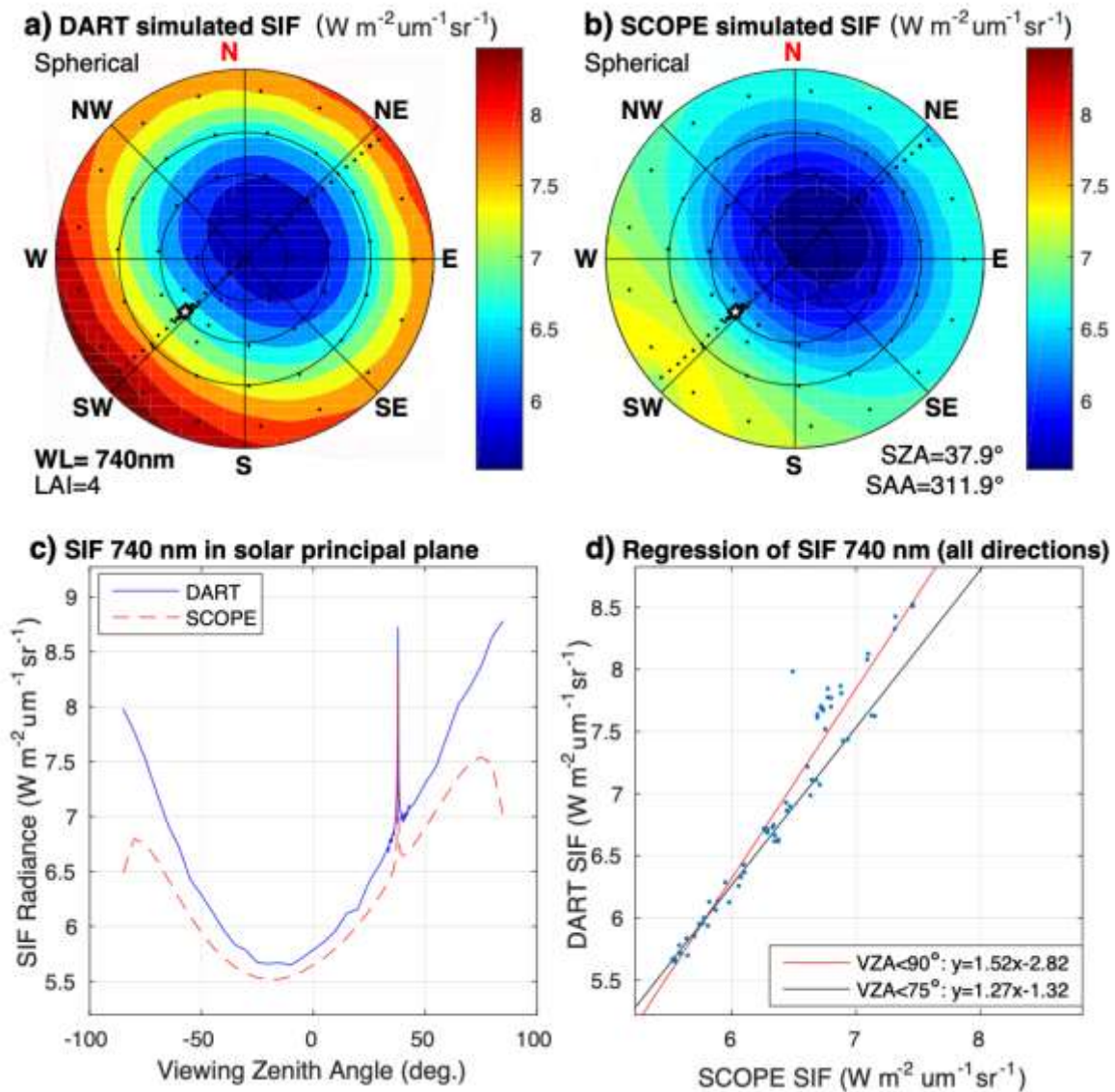
882 Figure A3. DART and mSCOPE nadir SIF of vegetation canopies simulated with the Spherical LAD,  
 883 three soils ( $\rho = 0\%$ ,  $\rho = 50\%$ ,  $\rho =$  loamy dark gravel soil) in two layers a) without and b) with energy  
 884 balance, and in three layers c) without and d) with energy balance (for abbreviations see Figure A2).



885

886 Figure A4. Best agreement when comparing a) DART and b) SCOPE multi-angular SIF of a turbid  
 887 medium canopy was found for the Erectophile LAD and a null soil reflectance. SIF radiance in the solar  
 888 principal plane and linear regression of turbid-like DART and turbid SCOPE simulations ( $R^2 = 0.99$ ,  
 889 RMSE = 0.03,  $d = 1.0$  for all simulated viewing directions, i.e.,  $VZA < 90^\circ$ , and RMSE = 0.02 for  
 890  $VZA < 75^\circ$ ) are shown in c) and d) graphs, respectively (for abbreviations and symbols see Figure 5).

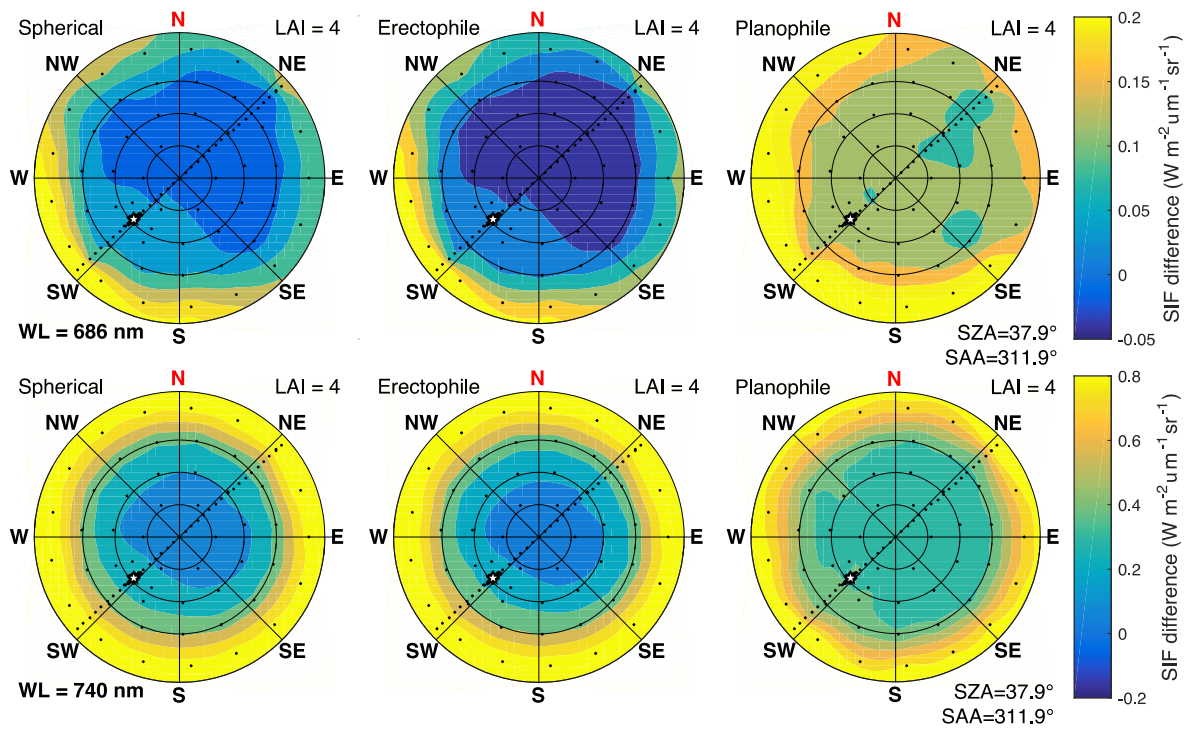




891

892 Figure A5. Worst agreement when comparing a) DART and b) SCOPE multi-angular SIF of turbid  
 893 medium canopy with the Spherical LAD and a 50% reflective soil. SIF radiance in the solar principal  
 894 plane and linear regression of turbid-like DART and turbid SCOPE simulations ( $R^2 = 0.94$ , RMSE =  
 895 0.21,  $d = 1.0$  for  $VZA < 90^\circ$  and  $R^2 = 0.99$ , RMSE = 0.07 for  $VZA < 75^\circ$ ) are shown in c) and d) graphs,  
 896 respectively (for abbreviations and symbols see Figure 5).

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897

898 Figure A6. DART-SCOPE differences in multi-angular SIF radiance at 686 and 740 nm for a canopy  
 899 with LAI = 4, having Spherical, Erectophile and Planophile LADs (the white star shows the solar  
 900 position and black dots indicate the simulated viewing directions; for abbreviations see Figure 5).

901

### 902 References

- 903 Aasen, H., Van Wittenberghe, S., Sabater Medina, N., Damm, A., Goulas, Y., Wieneke, S.,  
 904 Hueni, A., Malenovský, Z., Alonso, L., Pacheco-Labrador, J., Cendrero-Mateo, P.M.,  
 905 Tomelleri, E., Burkart, A., Cogliati, S., Rascher, U., & Mac Arthur, A. (2019). Sun-Induced  
 906 Chlorophyll Fluorescence II: Review of Passive Measurement Setups, Protocols, and Their  
 907 Application at the Leaf to Canopy Level. *Remote Sensing*, 11, 927
- 908 Ashley, M.D., & Rea, J. (1975). Seasonal vegetation differences from ERTS imagery. *Journal*  
 909 *of American Society of Photogrammetry*, 41, 713-719
- 910 Bendig, J., Malenovský, Z., Gautam, D., & Lucieer, A. (2020). Solar-Induced Chlorophyll  
 911 Fluorescence Measured From an Unmanned Aircraft System: Sensor Etaloning and  
 912 Platform Motion Correction. *IEEE Transactions on Geoscience and Remote Sensing*, 58,  
 913 3437-3444

- 914 Blair, B.O., & Baumgardner, M.F. (1977). Detection of the Green and Brown Wave in  
 915 Hardwood Canopy Covers Using Multidate, Multispectral Data from LANDSAT-11.  
 916 *Agronomy Journal*, 69, 808-811
- 917 Blender (2007). <https://www.blender.org/> (12 February 2020)
- 918 Chen, J.M., & Black, T.A. (1992). Defining leaf area index for non-flat leaves. *Plant, Cell &*  
 919 *Environment*, 15, 421-429
- 920 Croft, H., Chen, J.M., Wang, R., Mo, G., Luo, S., Luo, X., He, L., Gonsamo, A., Arabian, J.,  
 921 Zhang, Y., Simic-Milas, A., Noland, T.L., He, Y., Homolová, L., Malenovský, Z., Yi, Q.,  
 922 Beringer, J., Amiri, R., Hutley, L., Arellano, P., Stahl, C., & Bonal, D. (2020). The global  
 923 distribution of leaf chlorophyll content. *Remote Sensing of Environment*, 236, 111479
- 924 Danson, F.M. (1998). Teaching the physical principles of vegetation canopy reflectance using  
 925 the SAIL model. *Photogrammetric Engineering & Remote Sensing*, 64, 809-812
- 926 DART (2019).  
 927 [https://dart.omp.eu/Public/documentation/contenu/documentation/DART\\_handbook.pdf](https://dart.omp.eu/Public/documentation/contenu/documentation/DART_handbook.pdf)  
 928 (6 February 2020)
- 929 DART (2020).  
 930 [https://dart.omp.eu/Public/documentation/contenu/documentation/DART\\_User\\_Manual.p](https://dart.omp.eu/Public/documentation/contenu/documentation/DART_User_Manual.pdf)  
 931 [df](https://dart.omp.eu/Public/documentation/contenu/documentation/DART_User_Manual.pdf) (6 February 2020)
- 932 Féret, J.B., Berger, K., de Boissieu, F., & Malenovský, Z. (2020). PROSPECT-PRO for  
 933 estimating content of nitrogen-containing leaf proteins and other carbon-based  
 934 constituents. *Remote Sensing of Environment*, in review
- 935 Féret, J.B., Gitelson, A.A., Noble, S.D., & Jacquemoud, S. (2017). PROSPECT-D: Towards  
 936 modeling leaf optical properties through a complete lifecycle. *Remote Sensing of*  
 937 *Environment*, 193, 204-215
- 938 Frankenberg, C., Butz, A., & Toon, G.C. (2011). Disentangling chlorophyll fluorescence from  
 939 atmospheric scattering effects in O2 A-band spectra of reflected sun-light. *Geophysical*  
 940 *Research Letters*, 38
- 941 Gamon, J.A., Somers, B., Malenovský, Z., Middleton, E.M., Rascher, U., & Schaepman, M.E.  
 942 (2019). Assessing Vegetation Function with Imaging Spectroscopy. *Surveys in*  
 943 *Geophysics*, 40, 489-513
- 944 Gastellu-Etchegorry, J.-P., Wang, Y., Regaieg, O., Yin, T., Malenovský, Z., Zhen, Z., Yang,  
 945 X., Tao, Z., Landier, L., Al Bitar, A., Deschamps, A., Lauret, N., Guilleux, J., Chavanon,

## 2.1 VEGETATION SIMULATED AS FACETS

- 946 E., Cao, B., Qi, J., Kallel, A., Mitraka, Z., Chrysoulakis, N., Cook, B., & Morton, D. (2020).  
947 Recent improvements in the DART model for atmosphere, topography, large landscape,  
948 chlorophyll fluorescence, satellite image inversion. In, *IEEE International Geoscience and*  
949 *Remote Sensing Symposium* (p. 5). Virtual Symposium: IEEE
- 950 Gastellu-Etchegorry, J.-P., Yin, T., Lauret, N., Cajgfinger, T., Gregoire, T., Grau, E., Feret, J.-  
951 B., Lopes, M., Guilleux, J., Dedieu, G., Malenovský, Z., Cook, B., Morton, D., Rubio, J.,  
952 Durrieu, S., Cazanave, G., Martin, E., & Ristorcelli, T. (2015). Discrete Anisotropic  
953 Radiative Transfer (DART 5) for Modeling Airborne and Satellite Spectroradiometer and  
954 LIDAR Acquisitions of Natural and Urban Landscapes. *Remote Sensing*, 7, 1667-1701
- 955 Gastellu-Etchegorry, J.P. (2008). 3D modeling of satellite spectral images, radiation budget and  
956 energy budget of urban landscapes. *Meteorology and Atmospheric Physics*, 102, 187
- 957 Gastellu-Etchegorry, J.P., Demarez, V., Pinel, V., & Zagolski, F. (1996). Modeling radiative  
958 transfer in heterogeneous 3-D vegetation canopies. *Remote Sensing of Environment*, 58,  
959 131-156
- 960 Gastellu-Etchegorry, J.P., Lauret, N., Yin, T., Landier, L., Kallel, A., Malenovský, Z., Bitar,  
961 A.A., Aval, J., Benhmida, S., Qi, J., Medjdoub, G., Guilleux, J., Chavanon, E., Cook, B.,  
962 Morton, D., Chrysoulakis, N., & Mitraka, Z. (2017). DART: Recent Advances in Remote  
963 Sensing Data Modeling With Atmosphere, Polarization, and Chlorophyll Fluorescence.  
964 *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, 10,  
965 2640-2649
- 966 Gastellu-Etchegorry, J.P., Martin, E., & Gascon, F. (2004). DART: a 3D model for simulating  
967 satellite images and studying surface radiation budget. *International Journal of Remote*  
968 *Sensing*, 25, 73-96
- 969 Givnish, T.J. (1988). Adaptation to Sun and Shade: a Whole-Plant Perspective. *Functional*  
970 *Plant Biology*, 15, 63-92
- 971 Guan, K., Pan, M., Li, H., Wolf, A., Wu, J., Medvigy, D., Caylor, K.K., Sheffield, J., Wood,  
972 E.F., Malhi, Y., Liang, M., Kimball, J.S., Saleska, Scott R., Berry, J., Joiner, J., &  
973 Lyapustin, A.I. (2015). Photosynthetic seasonality of global tropical forests constrained by  
974 hydroclimate. *Nature Geoscience*, 8, 284-289
- 975 Guanter, L., Alonso, L., Gómez-Chova, L., Amorós-López, J., Vila, J., & Moreno, J. (2007).  
976 Estimation of solar-induced vegetation fluorescence from space measurements.  
977 *Geophysical Research Letters*, 34

- 978 Guanter, L., Zhang, Y., Jung, M., Joiner, J., Voigt, M., Berry, J.A., Frankenberg, C., Huete,  
 979 A.R., Zarco-Tejada, P., Lee, J.-E., Moran, M.S., Ponce-Campos, G., Beer, C., Camps-  
 980 Valls, G., Buchmann, N., Gianelle, D., Klumpp, K., Cescatti, A., Baker, J.M., & Griffis,  
 981 T.J. (2014). Global and time-resolved monitoring of crop photosynthesis with chlorophyll  
 982 fluorescence. *Proceedings of the National Academy of Sciences*, *111*, E1327-E1333
- 983 He, L., Chen, J.M., Liu, J., Mo, G., & Joiner, J. (2017). Angular normalization of GOME-2  
 984 Sun-induced chlorophyll fluorescence observation as a better proxy of vegetation  
 985 productivity. *Geophysical Research Letters*, *44*, 5691-5699
- 986 He, L., Magney, T., Dutta, D., Yin, Y., Köhler, P., Grossmann, K., Stutz, J., Dold, C., Hatfield,  
 987 J., Guan, K., Peng, B., & Frankenberg, C. (2020). From the Ground to Space: Using Solar-  
 988 Induced Chlorophyll Fluorescence to Estimate Crop Productivity. *Geophysical Research*  
 989 *Letters*, *47*, e2020GL087474
- 990 Hernández-Clemente, R., North, P.R.J., Hornero, A., & Zarco-Tejada, P.J. (2017). Assessing  
 991 the effects of forest health on sun-induced chlorophyll fluorescence using the  
 992 FluorFLIGHT 3-D radiative transfer model to account for forest structure. *Remote Sensing*  
 993 *of Environment*, *193*, 165-179
- 994 Hosgood, B., Jacquemoud, S., Andreoli, G., Verdebout, J., Pedrini, A., & Schmuck, G. (1994).  
 995 Leaf Optical Properties Experiment 93 (LOPEX93). In, *European Commission No. EUR*  
 996 *16095 EN*. Joint Research Centre, Institute for Remote Sensing Applications
- 997 Jacquemoud, S., & Baret, F. (1990). PROSPECT: A model of leaf optical properties spectra.  
 998 *Remote Sensing of Environment*, *34*, 75-91
- 999 Janoutová, R., Homolová, L., Malenovský, Z., Hanuš, J., Lauret, N., & Gastellu-Etchegorry,  
 1000 J.-P. (2019). Influence of 3D Spruce Tree Representation on Accuracy of Airborne and  
 1001 Satellite Forest Reflectance Simulated in DART. *Forests*, *10*, 292
- 1002 Joiner, J., Yoshida, Y., Vasilkov, A.P., Yoshida, Y., Corp, L.A., & Middleton, E.M. (2011).  
 1003 First observations of global and seasonal terrestrial chlorophyll fluorescence from space.  
 1004 *Biogeosciences*, *8*, 637-651
- 1005 Kallel, A. (2020). FluLCVRT: Reflectance and fluorescence of leaf and canopy modeling based  
 1006 on Monte Carlo vector radiative transfer simulation. *Journal of Quantitative Spectroscopy*  
 1007 *and Radiative Transfer*, *253*, 107183
- 1008 Kallel, A., & Nilson, T. (2013). Revisiting the vegetation hot spot modeling: Case of  
 1009 Poisson/Binomial leaf distributions. *Remote Sensing of Environment*, *130*, 188-204

## 2.1 VEGETATION SIMULATED AS FACETS

- 1010 Köhler, P., Guanter, L., Kobayashi, H., Walther, S., & Yang, W. (2018). Assessing the potential  
1011 of sun-induced fluorescence and the canopy scattering coefficient to track large-scale  
1012 vegetation dynamics in Amazon forests. *Remote Sensing of Environment*, 204, 769-785
- 1013 Leuning, R., Kelliher, F.M., De Pury, D.G.G., & Schulze, E.D. (1995). Leaf nitrogen,  
1014 photosynthesis, conductance and transpiration: scaling from leaves to canopies. *Plant, Cell  
1015 & Environment*, 18, 1183-1200
- 1016 Liu, W., Atherton, J., Möttus, M., Gastellu-Etchegorry, J.-P., Malenovský, Z., Raunonen, P.,  
1017 Åkerblom, M., Mäkipää, R., & Porcar-Castell, A. (2019a). Simulating solar-induced  
1018 chlorophyll fluorescence in a boreal forest stand reconstructed from terrestrial laser  
1019 scanning measurements. *Remote Sensing of Environment*, 232, 111274
- 1020 Liu, X., Guanter, L., Liu, L., Damm, A., Malenovský, Z., Rascher, U., Peng, D., Du, S., &  
1021 Gastellu-Etchegorry, J.-P. (2019b). Downscaling of solar-induced chlorophyll  
1022 fluorescence from canopy level to photosystem level using a random forest model. *Remote  
1023 Sensing of Environment*, 231, 110772
- 1024 Malenovský, Z., Homolová, L., Lukeš, P., Buddenbaum, H., Verrelst, J., Alonso, L.,  
1025 Schaepman, M.E., Lauret, N., & Gastellu-Etchegorry, J.-P. (2019). Variability and  
1026 Uncertainty Challenges in Scaling Imaging Spectroscopy Retrievals and Validations from  
1027 Leaves Up to Vegetation Canopies. *Surveys in Geophysics*, 40, 631-656
- 1028 Malenovský, Z., Homolová, L., Zurita-Milla, R., Lukeš, P., Kaplan, V., Hanuš, J., Gastellu-  
1029 Etchegorry, J.-P., & Schaepman, M.E. (2013). Retrieval of spruce leaf chlorophyll content  
1030 from airborne image data using continuum removal and radiative transfer. *Remote Sensing  
1031 of Environment*, 131, 85-102
- 1032 Malenovský, Z., Martin, E., Homolová, L., Gastellu-Etchegorry, J.-P., Zurita-Milla, R.,  
1033 Schaepman, M.E., Pokorný, R., Clevers, J.G.P.W., & Cudlín, P. (2008). Influence of  
1034 woody elements of a Norway spruce canopy on nadir reflectance simulated by the DART  
1035 model at very high spatial resolution. *Remote Sensing of Environment*, 112, 1-18
- 1036 Malenovský, Z., Ufer, C., Lhotáková, Z., Clevers, J.G.P.W., Schaepman, M.E., Albrechtová,  
1037 J., & Cudlín, P. (2006). A new hyperspectral index for chlorophyll estimation of a forest  
1038 canopy: Area under curve normalised to maximal band depth between 650-725 nm *EARSel  
1039 eProceedings*, 5, 161-172
- 1040 Migliavacca, M., Perez-Priego, O., Rossini, M., El-Madany, T.S., Moreno, G., van der Tol, C.,  
1041 Rascher, U., Berninger, A., Bessenbacher, V., Burkart, A., Carrara, A., Fava, F., Guan,

- 1042 J.H., Hammer, T.W., Henkel, K., Juarez-Alcalde, E., Julitta, T., Kolle, O., Martín, M.P.,  
 1043 Musavi, T., Pacheco-Labrador, J., Pérez-Burgueño, A., Wutzler, T., Zaehle, S., &  
 1044 Reichstein, M. (2017). Plant functional traits and canopy structure control the relationship  
 1045 between photosynthetic CO<sub>2</sub> uptake and far-red sun-induced fluorescence in a  
 1046 Mediterranean grassland under different nutrient availability. *New Phytologist*, 214, 1078-  
 1047 1091
- 1048 Mohammed, G.H., Colombo, R., Middleton, E.M., Rascher, U., van der Tol, C., Nedbal, L.,  
 1049 Goulas, Y., Pérez-Priego, O., Damm, A., Meroni, M., Joiner, J., Cogliati, S., Verhoef, W.,  
 1050 Malenovský, Z., Gastellu-Etchegorry, J.-P., Miller, J.R., Guanter, L., Moreno, J., Moya, I.,  
 1051 Berry, J.A., Frankenberg, C., & Zarco-Tejada, P.J. (2019). Remote sensing of solar-  
 1052 induced chlorophyll fluorescence (SIF) in vegetation: 50 years of progress. *Remote Sensing*  
 1053 *of Environment*, 231, 111177
- 1054 Myneni, R.B., & Ross, J. (2012). *Photon-Vegetation Interactions: Applications in Optical*  
 1055 *Remote Sensing and Plant Ecology*. Springer Berlin Heidelberg
- 1056 Niinemets, Ü., Keenan, T.F., & Hallik, L. (2015). A worldwide analysis of within-canopy  
 1057 variations in leaf structural, chemical and physiological traits across plant functional types.  
 1058 *New Phytologist*, 205, 973-993
- 1059 NOAA, NASA, & Air-Force, U.S. (1976). *U.S. Standard Atmosphere, 1976*. Washington D.C.:  
 1060 NOAA, U.S. Government Printing Office
- 1061 Nobel, P.S. (1976). Photosynthetic Rates of Sun versus Shade Leaves of *Hyptis emoryi* Torr.  
 1062 *Plant Physiology*, 58, 218-223
- 1063 North, P.R.J. (1996). Three-dimensional forest light interaction model using a monte carlo  
 1064 method. *IEEE Transactions on Geoscience and Remote Sensing*, 34, 946-956
- 1065 Pacheco-Labrador, J., Perez-Priego, O., El-Madany, T.S., Julitta, T., Rossini, M., Guan, J.,  
 1066 Moreno, G., Carvalhais, N., Martín, M.P., Gonzalez-Cascon, R., Kolle, O., Reischtein, M.,  
 1067 van der Tol, C., Carrara, A., Martini, D., Hammer, T.W., Moossen, H., & Migliavacca, M.  
 1068 (2019). Multiple-constraint inversion of SCOPE. Evaluating the potential of GPP and SIF  
 1069 for the retrieval of plant functional traits. *Remote Sensing of Environment*, 234, 111362
- 1070 Pedrós, R., Goulas, Y., Jacquemoud, S., Louis, J., & Moya, I. (2010). FluorMODleaf: A new  
 1071 leaf fluorescence emission model based on the PROSPECT model. *Remote Sensing of*  
 1072 *Environment*, 114, 155-167

## 2.1 VEGETATION SIMULATED AS FACETS

- 1073 Peng, B., Guan, K., Zhou, W., Jiang, C., Frankenberg, C., Sun, Y., He, L., & Köhler, P. (2020).  
1074 Assessing the benefit of satellite-based Solar-Induced Chlorophyll Fluorescence in crop  
1075 yield prediction. *International Journal of Applied Earth Observation and Geoinformation*,  
1076 90, 102126
- 1077 Pradal, C., Dufour-Kowalski, S., Boudon, F., Fournier, C., & Godin, C. (2008). OpenAlea: a  
1078 visual programming and component-based software platform for plant modelling.  
1079 *Functional Plant Biology*, 35, 751-760
- 1080 Rosema, A., Verhoef, W., Schroote, J., & Snel, J.F.H. (1991). Simulating fluorescence light-  
1081 canopy interaction in support of laser-induced fluorescence measurements. *Remote Sensing*  
1082 *of Environment*, 37, 117-130
- 1083 Sakai, Y., Kobayashi, H., & Kato, T. (2020). FLiES-SIF ver. 1.0: Three-dimensional radiative  
1084 transfer model for estimating solar induced fluorescence. *Geosci. Model Dev. Discuss.*,  
1085 2020, 1-36
- 1086 Sloup, P. (2013). [https://is.muni.cz/th/325196/fi\\_m/?lang=en](https://is.muni.cz/th/325196/fi_m/?lang=en) (18 February 2020)
- 1087 Sušila, P., & Nauš, J. (2007). A Monte Carlo study of the chlorophyll fluorescence emission  
1088 and its effect on the leaf spectral reflectance and transmittance under various conditions.  
1089 *Photochemical & Photobiological Sciences*, 6, 894-902
- 1090 Tong, C., Bao, Y., Zhao, F., Fan, C., Li, Z., & Huang, Q. (2021). Evaluation of the FluorWPS  
1091 Model and Study of the Parameter Sensitivity for Simulating Solar-Induced Chlorophyll  
1092 Fluorescence. *Remote Sensing*, 13
- 1093 van der Tol, C., Rossini, M., Cogliati, S., Verhoef, W., Colombo, R., Rascher, U., &  
1094 Mohammed, G. (2016). A model and measurement comparison of diurnal cycles of sun-  
1095 induced chlorophyll fluorescence of crops. *Remote Sensing of Environment*, 186, 663-677
- 1096 van der Tol, C., Verhoef, W., Timmermans, J., Verhoef, A., & Su, Z. (2009). An integrated  
1097 model of soil-canopy spectral radiances, photosynthesis, fluorescence, temperature and  
1098 energy balance. *Biogeosciences*, 6, 3109-3129
- 1099 van der Tol, C., Vilfan, N., Dauwe, D., Cendrero-Mateo, M.P., & Yang, P. (2019). The  
1100 scattering and re-absorption of red and near-infrared chlorophyll fluorescence in the  
1101 models Fluspect and SCOPE. *Remote Sensing of Environment*, 232, 111292
- 1102 Verhoef, W. (1984). Light scattering by leaf layers with application to canopy reflectance  
1103 modeling: The SAIL model. *Remote Sensing of Environment*, 16, 125-141



- 1104 Verrelst, J., Malenovský, Z., Van der Tol, C., Camps-Valls, G., Gastellu-Etchegorry, J.-P.,  
 1105 Lewis, P., North, P., & Moreno, J. (2019). Quantifying Vegetation Biophysical Variables  
 1106 from Imaging Spectroscopy Data: A Review on Retrieval Methods. *Surveys in Geophysics*,  
 1107 40, 589-629
- 1108 Verrelst, J., & Rivera, J.P. (2017). Chapter 16 - A Global Sensitivity Analysis Toolbox to  
 1109 Quantify Drivers of Vegetation Radiative Transfer Models. In G.P. Petropoulos, & P.K.  
 1110 Srivastava (Eds.), *Sensitivity Analysis in Earth Observation Modelling* (pp. 319-339):  
 1111 Elsevier
- 1112 Verrelst, J., Schaepman, M.E., Malenovský, Z., & Clevers, J.G.P.W. (2010). Effects of woody  
 1113 elements on simulated canopy reflectance: Implications for forest chlorophyll content  
 1114 retrieval. *Remote Sensing of Environment*, 114, 647-656
- 1115 Verroust, A., & Lazarus, F. (1999). Extracting skeletal curves from 3D scattered data. In,  
 1116 *Proceedings Shape Modeling International '99. International Conference on Shape*  
 1117 *Modeling and Applications* (pp. 194-201)
- 1118 Vilfan, N., van der Tol, C., Muller, O., Rascher, U., & Verhoef, W. (2016). Fluspect-B: A model  
 1119 for leaf fluorescence, reflectance and transmittance spectra. *Remote Sensing of*  
 1120 *Environment*, 186, 596-615
- 1121 Vilfan, N., van der Tol, C., & Verhoef, W. (2019). Estimating photosynthetic capacity from  
 1122 leaf reflectance and Chl fluorescence by coupling radiative transfer to a model for  
 1123 photosynthesis. *New Phytologist*, 223, 487-500
- 1124 Vilfan, N., Van der Tol, C., Yang, P., Wyber, R., Malenovský, Z., Robinson, S.A., & Verhoef,  
 1125 W. (2018). Extending Fluspect to simulate xanthophyll driven leaf reflectance dynamics.  
 1126 *Remote Sensing of Environment*, 211, 345-356
- 1127 Wang, C., Guan, K., Peng, B., Chen, M., Jiang, C., Zeng, Y., Wu, G., Wang, S., Wu, J., Yang,  
 1128 X., Frankenberg, C., Köhler, P., Berry, J., Bernacchi, C., Zhu, K., Alden, C., & Miao, G.  
 1129 (2020). Satellite footprint data from OCO-2 and TROPOMI reveal significant spatio-  
 1130 temporal and inter-vegetation type variabilities of solar-induced fluorescence yield in the  
 1131 U.S. Midwest. *Remote Sensing of Environment*, 241, 111728
- 1132 Widlowski, J.-L., Mio, C., Disney, M., Adams, J., Andredakis, I., Atzberger, C., Brennan, J.,  
 1133 Busetto, L., Chelle, M., Ceccherini, G., Colombo, R., Côté, J.-F., Eemäe, A., Essery, R.,  
 1134 Gastellu-Etchegorry, J.-P., Gobron, N., Grau, E., Haverd, V., Homolová, L., Huang, H.,  
 1135 Hunt, L., Kobayashi, H., Koetz, B., Kuusk, A., Kuusk, J., Lang, M., Lewis, P.E., Lovell,

## 2.1 VEGETATION SIMULATED AS FACETS

- 1136 J.L., Malenovsky, Z., Meroni, M., Morsdorf, F., Möttus, M., Ni-Meister, W., Pinty, B.,  
1137 Rautiainen, M., Schlerf, M., Somers, B., Stuckens, J., Verstraete, M.M., Yang, W., Zhao,  
1138 F., & Zenone, T. (2015). The fourth phase of the radiative transfer model intercomparison  
1139 (RAMI) exercise: Actual canopy scenarios and conformity testing. *Remote Sensing of*  
1140 *Environment*, 169, 418-437
- 1141 Willmott, C.J. (1981). On the validation of models. *Physical Geography*, 2, 184-194
- 1142 Wyber, R., Malenovsky, Z., Ashcroft, M., Osmond, B., & Robinson, S. (2017). Do Daily and  
1143 Seasonal Trends in Leaf Solar Induced Fluorescence Reflect Changes in Photosynthesis,  
1144 Growth or Light Exposure? *Remote Sensing*, 9, 604
- 1145 Yang, P., Prikaziuk, E., Verhoef, W., & van der Tol, C. (2020a). SCOPE 2.0: A model to  
1146 simulate vegetated land surface fluxes and satellite signals. *Geosci. Model Dev. Discuss.*,  
1147 2020, 1-26
- 1148 Yang, P., & van der Tol, C. (2018). Linking canopy scattering of far-red sun-induced  
1149 chlorophyll fluorescence with reflectance. *Remote Sensing of Environment*, 209, 456-467
- 1150 Yang, P., van der Tol, C., Campbell, P.K.E., & Middleton, E.M. (2020b). Fluorescence  
1151 Correction Vegetation Index (FCVI): A physically based reflectance index to separate  
1152 physiological and non-physiological information in far-red sun-induced chlorophyll  
1153 fluorescence. *Remote Sensing of Environment*, 240, 111676
- 1154 Yang, P., Verhoef, W., & van der Tol, C. (2017). The mSCOPE model: A simple adaptation to  
1155 the SCOPE model to describe reflectance, fluorescence and photosynthesis of vertically  
1156 heterogeneous canopies. *Remote Sensing of Environment*, 201, 1-11
- 1157 Yin, T., Gastellu-Etchegorry, J.-P., Lauret, N., Grau, E., & Rubio, J. (2013). A new approach  
1158 of direction discretization and oversampling for 3D anisotropic radiative transfer modeling.  
1159 *Remote Sensing of Environment*, 135, 213-223
- 1160 Zeng, Y., Badgley, G., Dechant, B., Ryu, Y., Chen, M., & Berry, J.A. (2019). A practical  
1161 approach for estimating the escape ratio of near-infrared solar-induced chlorophyll  
1162 fluorescence. *Remote Sensing of Environment*, 232, 111209
- 1163 Zhang, Z., Zhang, Y., Porcar-Castell, A., Joiner, J., Guanter, L., Yang, X., Migliavacca, M., Ju,  
1164 W., Sun, Z., Chen, S., Martini, D., Zhang, Q., Li, Z., Cleverly, J., Wang, H., & Goulas, Y.  
1165 (2020). Reduction of structural impacts and distinction of photosynthetic pathways in a  
1166 global estimation of GPP from space-borne solar-induced chlorophyll fluorescence.  
1167 *Remote Sensing of Environment*, 240, 111722

- 1168 Zhao, F., Dai, X., Verhoef, W., Guo, Y., van der Tol, C., Li, Y., & Huang, Y. (2016). FluorWPS:  
1169 A Monte Carlo ray-tracing model to compute sun-induced chlorophyll fluorescence of  
1170 three-dimensional canopy. *Remote Sensing of Environment*, 187, 385-399  
1171

## 2.2 Vegetation simulated as turbid medium

A DART turbid cell contains one or more types of turbid vegetation, and eventually, other scene elements made of facets. Leaves simulated as turbid medium are treated statistically using analytical equations that treat leaves as a whole and not as individual leaves. A type of turbid vegetation is characterized by a Leaf Angular Distribution (LAD)  $\frac{g(\theta_l)}{2\pi}$ , a leaf area volume density  $u_l$  ( $m^2/m^3$ ), and hemispherical spectral leaf optical properties (top side reflectance  $\rho_{top}$  and transmittance  $\tau_{top}$ , bottom side reflectance  $\rho_{bot}$  and transmittance  $\tau_{bot}$ ).

### 2.2.1 Modeling approach

#### *First order scattering and SIF emission*

A source radiation vector  $W_{in}(\lambda, \Omega_s)$  incident in a direction  $\Omega_s$  that crosses a turbid cell (*i.e.*, voxel) (Figure 2-1) is partly intercepted and partly transmitted. Its intercepted part is:

$$W_{int}(\lambda, \Omega_s) = W_{in}(\lambda, \Omega_s) \cdot [1 - e^{-G(\Omega_s) \cdot u_l \cdot \Delta l(\Omega_s)}] \quad (2.1)$$

with  $G(\Omega_s) = \int_0^{\frac{\pi}{2}} \frac{g(\theta_l)}{2\pi} \int_0^{2\pi} |\Omega_l \cdot \Omega_s| \cdot d\varphi_l \cdot \sin\theta_l \cdot d\theta_l$  and  $\Delta l(\Omega_s)$  the path length of  $W_{in}(\lambda, \Omega_s)$  inside the cell.

Radiation intercepted by a turbid cell is either absorbed or scattered. The first order energy scattered in the discrete direction  $(\Omega_v, \Delta\Omega_v)$  due to the interception of  $W_{int}(\lambda, \Omega_s)$  is:

$$W_{1,scat}(\lambda, \Omega_s, \Omega_v, \Delta\Omega_v) = W_{in}(\lambda, \Omega_s) \cdot T_{scat}(\lambda, \Omega_s, \Omega_v, \Delta\Omega_v) \quad (2.2)$$

with  $T_{scat}(\lambda, \Omega_s, \Omega_v, \Delta\Omega_v)$  the scattering transfer function:

$$T_{scat}(\lambda, \Omega_s, \Omega_v, \Delta\Omega_v) = \sum_{\theta_{l,i}} \frac{g(\theta_{l,i})}{2\pi} \sum_{\varphi_{l,i}} \frac{\alpha_\lambda}{\pi} |\Omega_{l,ij} \cdot \Omega_s| \cdot |\Omega_{l,ij} \cdot \Omega_v| \Delta\varphi_{l,j} \sin\theta_{l,i} \Delta\theta_{l,i} \frac{\Delta\Omega_v}{G(\Omega_s)} \quad (2.3)$$

$$\alpha_\lambda = \begin{cases} \rho_{top} & \text{if } \Omega_{l,ij} \cdot \Omega_s < 0 \text{ and } \Omega_{l,ij} \cdot \Omega_v > 0 \\ \tau_{top} & \text{if } \Omega_{l,ij} \cdot \Omega_s < 0 \text{ and } \Omega_{l,ij} \cdot \Omega_v < 0 \\ \rho_{bot} & \text{if } \Omega_{l,ij} \cdot \Omega_s > 0 \text{ and } \Omega_{l,ij} \cdot \Omega_v < 0 \\ \tau_{bot} & \text{if } \Omega_{l,ij} \cdot \Omega_s > 0 \text{ and } \Omega_{l,ij} \cdot \Omega_v > 0 \end{cases}$$

In presence of SIF emission, any radiation vector has 3 components: total, PSI and PSII radiation. SIF emission and radiation scattering are computed in each discrete direction. SIF excitation-emission matrices play a role for SIF emission similar to that of leaf reflectance and transmittance for scattering. SIF emission at spectral band  $(\lambda_w, \Delta\lambda_w)$  in the discrete direction  $(\Omega_v, \Delta\Omega_v)$ , by the photosystem  $x$  (*i.e.*, 1 or 2), due to the intercepted radiation  $W_{int}(\lambda_u, \Omega_s)$  at spectral band  $(\lambda_u, \Delta\lambda_u)$  is:

$$W_{PSx}(\lambda_u \rightarrow \lambda_w, \Omega_s, \Omega_v, \Delta\Omega_v) = W_{in}(\lambda_u, \Omega_s) \cdot T_{PSx}(\lambda_u, \lambda_w, \Omega_s, \Omega_v, \Delta\Omega_v) \quad (2.4)$$

with  $T_{PSx}(\lambda_u, \lambda_w, \Omega_s, \Omega_v, \Delta\Omega_v)$  the fluorescence transfer function:

$$T_{PSx}(\lambda_u, \lambda_w, \Omega_s, \Omega_v, \Delta\Omega_v) = \sum_{\theta_{l,i}} \frac{g(\theta_{l,i})}{2\pi} \sum_{\varphi_{l,i}} \frac{M_{xyuv}}{\pi} |\Omega_{l,ij} \cdot \Omega_s| \cdot |\Omega_{l,ij} \cdot \Omega_v| \Delta\varphi_{l,j} \sin \theta_{l,i} \Delta\theta_{l,i} \frac{\Delta\Omega_v}{G(\Omega_s)} \quad (2.5)$$

$$M_{xyuv} = \begin{cases} M_{x,backward,u,w}^{top} & \text{if } \Omega_{l,ij} \cdot \Omega_s < 0 \text{ and } \Omega_{l,ij} \cdot \Omega_v > 0 \\ M_{x,forward,u,w}^{top} & \text{if } \Omega_{l,ij} \cdot \Omega_s < 0 \text{ and } \Omega_{l,ij} \cdot \Omega_v < 0 \\ M_{x,backward,u,w}^{bot} & \text{if } \Omega_{l,ij} \cdot \Omega_s > 0 \text{ and } \Omega_{l,ij} \cdot \Omega_v < 0 \\ M_{x,forward,u,w}^{bot} & \text{if } \Omega_{l,ij} \cdot \Omega_s > 0 \text{ and } \Omega_{l,ij} \cdot \Omega_v > 0 \end{cases}$$

The first order SIF emission at the spectral band  $(\lambda_w, \Delta\lambda_w)$  is the sum of the contribution of all the excitation spectral bands to the emission in this band.

$$W_{1,PSx}(\lambda_w, \Omega_s, \Omega_v, \Delta\Omega_v) = \sum_u W_{PSx}(\lambda_u \rightarrow \lambda_w, \Omega_s, \Omega_v, \Delta\Omega_v) \quad (2.6)$$

### **Transmission and interception of first order rays**

$W_{1,scat}(\lambda, \Omega_s, \Omega_v, \Delta\Omega_v)$  and  $W_{1,PSx}(\lambda_w, \Omega_s, \Omega_v, \Delta\Omega_v)$  are partly transmitted through the cell along the path  $\Delta l(M, \Omega_v)$  between the emission point M and the cell border and give:

- The first order scattered flux and SIF flux that exit the cells in the direction  $(\Omega_v, \Delta\Omega_v)$ :

$$W_{1,scat,\alpha}(\lambda, \Omega_s, \Omega_v, \Delta\Omega_v) = W_{1,scat}(\lambda, \Omega_s, \Omega_v, \Delta\Omega_v) \cdot e^{-G(\Omega_s) \cdot u_l \cdot \Delta l(M, \Omega_v)} \quad (2.7)$$

$$W_{1,PSx,\alpha}(\lambda_w, \Omega_s, \Omega_v, \Delta\Omega_v) = W_{1,PSx}(\lambda_w, \Omega_s, \Omega_v, \Delta\Omega_v) \cdot e^{-G(\Omega_s) \cdot u_l \cdot \Delta l(M, \Omega_v)} \quad (2.8)$$

- The associated total and SIF intercepted fluxes in the cell in all directions are:

## 2.2 VEGETATION SIMULATED AS TURBID MEDIUM

$$W_{1,int,1}(\lambda, \Omega_s) = \sum_v W_{1,scat}(\lambda, \Omega_s, \Omega_v, \Delta\Omega_v) \cdot (1 - e^{-G(\Omega_s) \cdot u_l \cdot \Delta l(M, \Omega_v)}) \quad (2.9)$$

$$W_{1,PSx,int,1}(\lambda_w, \Omega_s) = \sum_v W_{1,PSx}(\lambda_w, \Omega_s, \Omega_v, \Delta\Omega_v) \cdot (1 - e^{-G(\Omega_s) \cdot u_l \cdot \Delta l(M, \Omega_v)}) \quad (2.10)$$

### *Within cell multiple scattering and SIF emission*

The intercepted flux  $W_{1,int,1}(\lambda, \Omega_s)$  is scattered and partly transmitted, then partly intercepted, and so on. Assuming the isotropy of the within cell scattered rays, the multiple scattered flux that escapes the cell is:

$$\begin{aligned} W_{1,int,\beta}(\lambda, \Omega_s) &= W_{1,int,1}(\lambda, \Omega_s) \cdot [\omega \bar{T} + \omega \bar{T}(\omega - \omega \bar{T}) + \omega \bar{T}(\omega - \omega \bar{T})^2 + \dots] \quad (2.11) \\ &= W_{1,int,1}(\lambda, \Omega_s) \cdot \frac{\omega \bar{T}}{[1 - \omega(1 - \bar{T})]} \end{aligned}$$

with  $\omega$  the leaf single scattering albedo and  $\bar{T}$  the mean cell transmittance along the paths  $\Delta l(M, \Omega_v)$  from the cell center to the cell faces:

$$\bar{T} = \frac{1}{4\pi} \int_{4\pi} e^{-G(\Omega_v) \cdot u_l \cdot \Delta l(M, \Omega_v)} \cdot d\Omega_v \quad (2.12)$$

Similarly, for the SIF energy:

$$W_{1,PSx,int,\beta}(\lambda_w, \Omega_s) = W_{1,PSx,int,1}(\lambda_w, \Omega_s) \cdot \frac{\omega_w \bar{T}}{[1 - \omega_w(1 - \bar{T})]} \quad (2.13)$$

The propagation of  $W_{1,int,1}(\lambda, \Omega_s)$  in the cell after multiple scattering gives rise to absorption:

$$\begin{aligned} W_{1,abs}(\lambda, \Omega_s) &= W_{1,int,1}(\lambda, \Omega_s) - W_{1,int,\beta}(\lambda, \Omega_s) \quad (2.14) \\ &= W_{1,int,1}(\lambda, \Omega_s) \cdot \frac{1 - \omega \bar{T}}{[1 - \omega(1 - \bar{T})]} \end{aligned}$$

Similarly, for the SIF energy:

$$W_{1,PSx,abs}(\lambda, \Omega_s) = W_{1,PSx,int,1}(\lambda_w, \Omega_s) \cdot \frac{1 - \omega_w \bar{T}}{[1 - \omega_w(1 - \bar{T})]} \quad (2.15)$$

Therefore, the propagation of  $W_{1,int,1}(\lambda, \Omega_s)$  gives also rise to new SIF emission:

$$W_{1,int,PSx}(\lambda_w, \Omega_s) = \sum_u 2 \cdot \frac{W_{1,abs}(\lambda_w, \Omega_s)}{1 - \omega_u} \cdot M_{xuv} \quad (2.16)$$

$$\text{where } M_{xuv} = \frac{M_{x,forward,uv}^{top} + M_{x,backward,uv}^{top} + M_{x,forward,uv}^{bot} + M_{x,backward,uv}^{bot}}{4}$$

Part of this emitted SIF exits the cell directly, or after simple or multiple scattering:

$$\begin{aligned} W_{1,int,PSx,\gamma}(\lambda_w, \Omega_s) &= W_{1,int,PSx}(\lambda_w, \Omega_s) \cdot [\bar{T} + \omega\bar{T}(1 - \bar{T}) + \omega^2 \cdot \bar{T}(1 - \bar{T})^2 + \dots] \quad (2.17) \\ &= W_{1,int,PSx}(\lambda_w, \Omega_s) \cdot \frac{\bar{T}}{[1 - \omega(1 - \bar{T})]} \end{aligned}$$

The SIF emitted in each direction is then:

$$W_{1,int,PSx,\gamma}(\lambda_w, \Omega_s \rightarrow \Omega_v) = W_{1,int,PSx,\gamma}(\lambda_w, \Omega_s) \cdot \xi(M, \Omega_v) \quad (2.18)$$

with

$$\xi(M, \Omega_v) = \frac{e^{-G(\Omega_v)u_l\Delta l(M, \Omega_v)} \cdot \int_{4\pi} \int_{2\pi} |\Omega_s \cdot \Omega_l| \frac{g(\theta_l)}{2\pi} f(\Omega_l, \Omega_s \rightarrow \Omega_v) d\Omega_l d\Omega_s d\Omega_v}{\int_{4\pi} e^{-G(\Omega_v)u_l\Delta l(M, \Omega_v)} \cdot \int_{4\pi} \int_{2\pi} |\Omega_s \cdot \Omega_l| \frac{g(\theta_l)}{2\pi} f(\Omega_l, \Omega_s \rightarrow \Omega_v) d\Omega_l d\Omega_s d\Omega_v} \quad (2.19)$$

The propagation of  $W_{1,int,PSx}$  in the cell can further give rise to absorption and SIF emission, which in turn can give rise to higher order SIF emissions. However, these SIF emissions are small enough to be neglected.

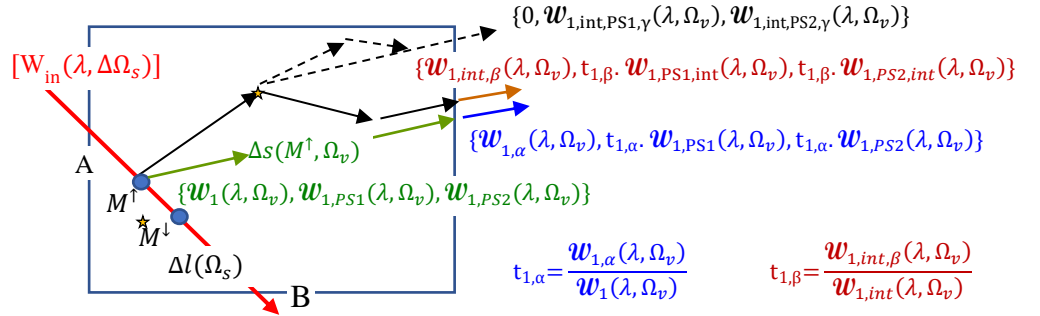


Figure 2-1: Incident source vector  $[W_{in}(\lambda, \Delta\Omega_s)]$  onto a turbid cell, with source points  $M^\uparrow$  and  $M^\downarrow$ , and energy  $\{W_1(\lambda, \Omega_v), W_{1,PS1}(\lambda, \Omega_v), W_{1,PS2}(\lambda, \Omega_v)\}$  from  $M^\uparrow$ .  $\Delta l(\Omega_s)$  is the distance between the entry A and exit B of the incident ray.  $\Delta s(M^\uparrow, \Omega_v)$  is the distance between  $M^\uparrow$  and the cell exit along direction  $\Omega_v$ .  $W_{1,\alpha}(\lambda, \Omega_v)$  is equal to the direct transmission of  $W_1(\lambda, \Omega_v)$  outside the cell without any scattering, whereas  $W_{1,int,\beta}(\lambda, \Omega_v)$  is the transmission of  $W_1(\lambda, \Omega_v)$  outside the cell with scattering events.

### $\eta$ factors

As for vegetation simulated as facets, the  $\eta$  factors simulated by SCOPE can be imported to scale the leaf-level SIF emission in order to consider the effects of local environment.

SCOPE computes two types of  $\eta$  factors:

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-  $\eta_{sunlit}(n, \theta_l, \varphi_l)$  for sunlit leaves at layer  $n$ , and leaves with a leaf zenith and azimuth angles  $\theta_l$  and  $\varphi_l$ , respectively. In this case, an average profile is computed for each layer:

$$\begin{aligned} \bar{\eta}_{sunlit}(n) &= \int_0^{2\pi} \int_0^{\frac{\pi}{2}} \eta_{sunlit}(n, \theta_l, \varphi_l) \cdot \frac{g(\theta_l)}{2\pi} \cdot \sin \theta_l \cdot d\theta_l \cdot d\varphi_l \\ &\approx \sum_{\varphi_l} \sum_{\theta_l} \eta_{sunlit}(n, \theta_l, \varphi_l) \cdot \frac{g(\theta_l)}{2\pi} \cdot \sin \theta_l \cdot \Delta\theta_l \cdot \Delta\varphi_l \end{aligned} \quad (2.20)$$

-  $\eta_{shaded}(n)$  for shaded cells at layer  $n$ . It is used as is.

The number of layers in the DART simulation and in the SCOPE imported  $\eta$  files usually differ. If the number of DART layers is lower, the corresponding layers of the  $\eta$  profile are averaged, if it is higher, the values of the  $\eta$  profiles are interpolated to provide a value for each layer.

### 2.2.2 Results

The accuracy of DART-FT modeling in turbid vegetation was tested by comparing it with DART-FT modeling in quasi-turbid vegetation, because the latter one has already been successfully tested with the SCOPE model. Figure 2-2 shows DART-FT SIF emission and nadir radiance for a homogeneous canopy simulated as turbid medium and quasi turbid medium. The agreement is very good for the two types of vegetation representation, with relative differences less than 0.1% for emitted SIF and less than 0.8% for radiance. The relative difference is lower for SIF emission than for SIF radiance because SIF radiance has an additional step from the emission to the top of canopy. The large absorption of SIF by the vegetation explains that the red peak of PSII is relatively smaller for SIF radiance than for SIF emission.

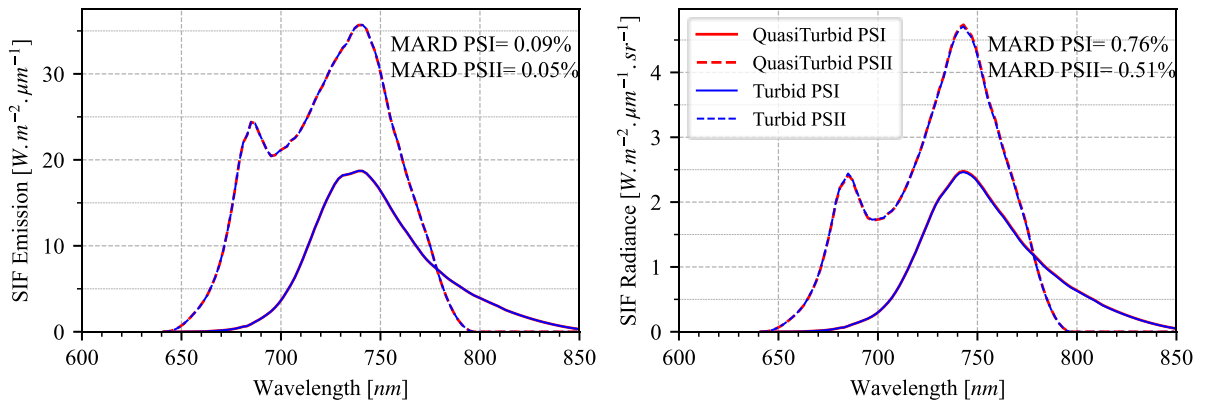


Figure 2-2: DART-FT SIF emission and nadir radiance for a homogeneous canopy simulated as turbid medium and quasi turbid medium.



## 2.3 Conclusion

In this chapter, the SIF modeling approaches in DART-FT were presented for facets-based and turbid-based vegetation. Up to now, the impact for the local climatology on the SIF emission can be considered only via the coupling with SCOPE 1D energy module. The results were in good agreement with the SCOPE/mSCOPE models. However, DART-FT requires very huge computation time and memory to simulate SIF for large scale scenes, which would be very important notably to simulate images of spaceborne sensors. For example, the spatial resolution of the FLEX satellite will be 300 m. Therefore, a more efficient modeling strategy is needed to meet these needs. This highlights the interest of the new Monte Carlo modeling strategy in DART-Lux because of its much better computational efficiency in terms of simulation time and memory. However, for this objective, the SIF modeling must be introduced in DART-Lux. This introduction is presented in the next chapter.

## Appendix 2-1: Nomenclature

Symbol	Description	Unit
$\frac{g(\theta)}{2\pi}$	Leaf angular distribution function	$sr^{-1}$
$G(\Omega_s)$	Mean projection of leaf normal on the direction $\Omega_s$	-
$\bar{T}$	Mean cell transmittance	-
$T_{PSx}(\lambda_u, \lambda_w, \Omega_s, \Omega_v, \Delta\Omega_v)$	Fluorescence transfer function: excitation band $u$ , emission band $w$ , incident direction $\Omega_s$ , outgoing direction $(\Omega_v, \Delta\Omega_v)$	-
$T_{scat}(\lambda, \Omega_s, \Omega_v, \Delta\Omega_v)$	Scattering transfer function: incident direction $\Omega_s$ , outgoing direction $(\Omega_v, \Delta\Omega_v)$	-
$W_{in}(\lambda, \Omega_s)$	Source vector of incident radiation in direction $\Omega_s$	$W \cdot \mu m^{-1}$
$W_{int}(\lambda, \Omega_s)$	Intercepted radiation from $W_{in}(\lambda, \Omega_s)$	$W \cdot \mu m^{-1}$
$W_{PSx}(\lambda_u \rightarrow \lambda_w, \Omega_s, \Omega_v, \Delta\Omega_v)$	First order SIF at photosystem $x$ and band $w$ due to excitation in band $u$	$W \cdot \mu m^{-1}$
$W_{1,scat}(\lambda, \Omega_s, \Omega_v, \Delta\Omega_v)$	First order scattering due to $W_{int}(\lambda, \Omega_s)$	$W \cdot \mu m^{-1}$
$W_{1,scat,\alpha}(\lambda, \Omega_s, \Omega_v, \Delta\Omega_v)$	Part of $W_{1,scat}$ that exits the cell	$W \cdot \mu m^{-1}$
$W_{1,int,\beta}(\lambda, \Omega_s)$	Part of $W_{1,int,1}$ that exits the cell after multiple scattering	$W \cdot \mu m^{-1}$
$W_{1,int,PSx}(\lambda_w, \Omega_s)$	SIF emission at photosystem $x$ due to the propagation of $W_{1,int,1}$	$W \cdot \mu m^{-1}$
$W_{1,int,1}(\lambda, \Omega_s)$	Intercepted part from first order scattered radiation	$W \cdot \mu m^{-1}$
$W_{1,abs}(\lambda, \Omega_s)$	Absorbed part from first order scattered radiation	$W \cdot \mu m^{-1}$
$W_{1,PSx}(\lambda_w, \Omega_s, \Omega_v, \Delta\Omega_v)$	First order SIF due to $W_{int}(\lambda, \Omega_s)$	$W \cdot \mu m^{-1}$
$W_{1,PSx,\alpha}(\lambda_w, \Omega_s, \Omega_v, \Delta\Omega_v)$	Part of $W_{1,PSx,\alpha}$ that exits the cell	$W \cdot \mu m^{-1}$

$W_{1,PSx,int,\beta}(\lambda_w, \Omega_s)$	Part of $W_{1,PSx,int,1}$ that exits the cell after multiple scattering	$W \cdot \mu m^{-1}$
$W_{1,PSx,int,1}(\lambda_w, \Omega_s)$	Interception due to first order SIF radiation	$W \cdot \mu m^{-1}$
$W_{1,PSx,abs}(\lambda, \Omega_s)$	Absorbed part from first order SIF radiation	$W \cdot \mu m^{-1}$
$W_{1,int,PSx,\gamma}(\lambda_w, \Omega_s)$	Part of $W_{1,int,PSx}$ that exits the cell after simple or multiple scattering	$W \cdot \mu m^{-1}$
$W_{1,int,PSx,\gamma}(\lambda_w, \Omega_s \rightarrow \Omega_v)$	Part of $W_{1,int,PSx,\gamma}$ that exits from direction $\Omega_v$	$W \cdot \mu m^{-1}$
$u_l$	Leaf volume density	$m^2 \cdot m^{-3}$
$\rho_{top} \tau_{top} \rho_{bot} \tau_{bot}$	Leaf top reflectance, top transmittance, bottom reflectance, bottom transmittance respectively	-
$\eta$	Fluorescence eta factor	-
$\xi(M, \Omega_v)$	Fraction of radiation scattered in direction $\Omega_v$	-
$\Delta l(\Omega_s)$	Path along $\Omega_s$	$m$

# Chapter 3

## **SIF modeling in DART-Lux**

DART-Lux is based on an adaptation of the LuxCoreRender opensource rendering software. A fundamental adaptation was to replace the RGB triple color channel hardly coded in this software, to multiband modeling to allow multispectral and hyperspectral simulations. This step was needed to simulate SIF because SIF modeling usually needs a large number of spectral bands at a fine spectral resolution over the whole SIF excitation and emission spectral domains. However, to simulate SIF emission, it is essential to have an interdependency between spectral bands as the excitation at a certain wavelength can induce fluorescence emission at other wavelengths, which is not possible using the original LuxCoreRender nor the first versions of DART-Lux. Moreover, the turbid medium is a representation of vegetation that is specific for remote sensing models and is not included in rendering software originally designed for other purposes. This chapter presents the new modeling that I designed and implemented into DART-Lux in order to solve these issues. The first section presents the SIF modeling for facets-based vegetation and all the consequent modeling adaptations that were made to allow DART-Lux to simulate SIF. An article describing the methodology and evaluating the accuracy of the SIF modeling in DART-Lux of which I am the first author has been submitted to the International Journal of Applied Earth Observation and Geoinformation. The second section presents first the turbid volume vegetation modeling in DART-Lux which was introduced by analogy to the fluids modeling. Then, the SIF modeling for turbid vegetation is introduced.

## 3.1 Vegetation simulated as facets

### 3.1.1 Modeling approach

The implementation of SIF emission in DART-Lux for vegetation simulated as facets also uses the fluorescence excitation-emission matrices computed by Fluspect and resampled to the user-defined DART bands. The same rule of covering all the excitation spectral interval (*i.e.*, [400 – 750 nm]) with non-overlapping bands applies. To include the SIF radiation, physical quantities in DART-Lux should have 3 components for total, PSI and PSII radiation. However, to evaluate the SIF radiance for light paths traced from the sensor (*i.e.*, in the backward direction), this is not sufficient. A higher dimensional representation needed to be introduced to account for the three components and all the possible interactions. The detailed description of this methodology and its implementation is available in a submitted paper (cf. Section 3.1.3).

### 3.1.2 Results

Model-to-model comparisons were used to evaluate the implementation of SIF in DART-Lux. Canopy SIF emission and radiance simulated by DART-Lux were compared to those simulated by DART-FT and SCOPE for different types of canopies. DART-Lux closely matched DART-FT in all configurations, with less than 2% of relative difference. It also matched SCOPE for homogeneous canopies, but not with 3D canopy (maize crop field) especially for oblique viewing directions. Computation time and memory requirements were usually lower than DART-FT. The gain in computational efficiency relative to DART-FT was systematically very large for large and complex scenes. However, this large gain decreased when the number of spectral bands increases. The theory of the new SIF modeling and results are detailed in a submitted paper (cf. Section 3.1.3).

### 3.1.3 Submitted article

## 1 **Bi-directional Monte-Carlo modelling of solar-induced chlorophyll** 2 **fluorescence images for 3D vegetation canopies in the DART model**

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### 7 **Abstract**

8 Remote sensing (RS) of solar-induced chlorophyll fluorescence (SIF) has a great potential  
9 for monitoring plant photosynthetic activity. Radiative transfer models (RTM) are essential to  
10 better interpret and extract information from SIF signals. DART is one of the most  
11 comprehensive and accurate 3D RTMs. Its standard mode DART-FT simulates SIF using a  
12 discrete ordinate method but is not adapted to large landscapes due to computational constraints.  
13 DART-Lux, the new mode based on a bi-directional path tracing algorithm, greatly improves  
14 DART computational efficiency for simulating images. This paper presents the theory of a  
15 novel SIF modelling algorithm in DART-Lux. We verified its accuracy with DART-FT and the  
16 SCOPE model for three types of canopies: turbid medium, maize field and forest. DART-Lux  
17 closely matches DART-FT (relative difference < 2%) with much better computational  
18 efficiency depending on the scene complexity, number of spectral bands and needed accuracy.  
19 For example, simulation time is reduced by a factor of  $\approx 48$ , and memory usage by  $\approx 50$  for a  
20 maize field at 1 cm resolution. It allowed to simulate SIF images of large scenes as the  
21  $3 \times 3 \text{ km}^2$  Ripperdan agricultural site that DART-FT could not simulate. The new SIF  
22 modelling algorithm opens new horizons for RS studies of large and complex landscapes. It is  
23 available as part of released DART versions (v1152 onwards) (<https://dart.omp.eu/>).

### 24 **Keywords**

25 SIF, Remote sensing, Bi-directional path tracing, 3D vegetation structure, DART

### 26 **I. Introduction**

27 Solar-induced fluorescence (SIF) of vegetation is a spontaneous radiation re-emission from  
28 640 to 850 nm due to absorbed sunlight from 400 to 750 nm. In competition with the  
29 photochemical and heat dissipation processes, it allows an electron from a chlorophyll  
30 molecule excited by absorbing a quantum of light, to dispose of its excess energy. It provides

31 valuable information on real-time plants photosynthetic activity (Mohammed et al., 2019)  
32 which enables early stress detection (Song et al., 2018) and gross primary production (GPP)  
33 estimation (Zhang et al., 2020).

34 The fluorescence quantum efficiency ( $fqe$ ) of chlorophyll in vivo does not exceed 10%, with  
35 typical values under steady-state illumination of 0.5–3% (Porcar-Castell et al., 2014). Hence,  
36 the SIF remote sensing (RS) signal is a small fraction of sunlight scattered by a vegetation  
37 canopy. The resulting difficulty in interpreting SIF RS signal in terms of vegetation functioning  
38 traits is largely amplified by the dependence of the SIF signal on the vegetation 3D structure,  
39 combined with illumination and observation conditions (Hornero et al., 2021; Regaieg et al.,  
40 2021). This stresses the importance of physical models to link the within canopy SIF emission  
41 with RS signals. An ideal radiative model of SIF includes two major sub-models: (1) Leaf SIF  
42 emission model considering the incident spectral irradiance, leaf structure and biochemistry,  
43 and the probability of a photon absorbed by photosystems I (PSI) and II (PSII) to be re-emitted  
44 as SIF (*i.e.*,  $fqe$ ) derived from leaf physiological modelling. (2) Radiative transfer (RT) model  
45 of the radiation propagation in the canopy to simulate the SIF radiance at the bottom and/or top  
46 of the atmosphere (*i.e.*, RS signal).

47 Here, we consider top of canopy SIF modelling including vegetation 3D architecture. Canopy  
48 SIF models are generally canopy reflectance models with an imbedded leaf-level fluorescence  
49 model. For example, FLSAIL (Rosema et al., 1991), FluorSAIL (Miller, 2005) and SCOPE  
50 (van der Tol et al., 2009) models combine leaf SIF modelling with the SAIL canopy reflectance  
51 model (Verhoef, 1984). SAIL is one-dimensional (1D), as it represents vegetation as  
52 superimposed homogeneous layers filled by a turbid medium: infinite number of infinitely  
53 small plane elements characterized by a statistical leaf angular distribution (LAD), a leaf area  
54 index (LAI), and optical properties. It simulates the radiative transfer with four streams: a  
55 source term for direct solar radiation, one stream for upward and one stream for downward  
56 fluxes, and scattered radiance is integrated along the observation direction. SCOPE is a  
57 reference model for 1D SIF modelling (Damm et al., 2015; Verrelst et al., 2019). The 1D  
58 models' major limitation is neglecting the vegetation horizontal heterogeneity. Accounting for  
59 vertical heterogeneity as in mSCOPE (Yang et al., 2017) only partly improves the situation.  
60 Indeed, the canopy horizontal heterogeneity has usually a much greater influence on RS signals  
61 than vertical heterogeneity (Regaieg et al., 2021). Some approaches aiming to simulate SIF at  
62 the global scale account for the influence of the canopy horizontal heterogeneity using clumping

### 3.1 VEGETATION SIMULATED AS FACETS

63 indices (Braghiere et al., 2021). However, they cannot fully capture the actual canopies 3D  
64 architecture including local topography, and the presence of woody elements, that impact  
65 remotely sensed SIF signals (Malenovský et al., 2021; Regaieg et al., 2021).

66 3D SIF RTMs adapted to realistic vegetation canopies descriptions represented as facets or 3D  
67 turbid medium are of great interest because of the 1D models limitation. For example, FLiES-  
68 SIF (Sakai et al., 2020) simulates SIF tree canopies having geometrically simple crowns (*e.g.*,  
69 cone, cylinder, spheroid) whereas FluorFLIGHT (Hernández-Clemente et al., 2017), FluorWPS  
70 (Zhao et al., 2016), DART (Malenovský et al., 2021) and FluCVRT (Kallel, 2020) simulate SIF  
71 for any canopy type. FluCVRT includes 3D leaf-level SIF modelling. These models use Monte  
72 Carlo ray tracing techniques, apart from DART that uses an adapted forward discrete ordinates  
73 method, called DART-FT (Flux Tracking). DART-FT simulates the canopy SIF radiance and  
74 reflectance images, the canopy 3D SIF radiative budget (RB) per photosystem, and therefore  
75 the canopy fluorescence escape factor (Guanter et al., 2014). DART-FT SIF modelling has been  
76 validated with model comparison (Malenovský et al., 2021), and successfully used in various  
77 SIF studies such as sensitivity analysis of the SIF signal in architecturally complex forest  
78 canopies (W. Liu et al., 2019; Malenovský et al., 2021), scaling canopy-level SIF down to  
79 photosystems level (X. Liu et al., 2019), and studying the far-red SIF escape probability from  
80 forest canopies (W. Liu et al., 2020).

81 Compared to 1D models, 3D models use more parameters, are more computationally  
82 demanding and therefore are not well adapted to regional or global scales. Indeed, forward  
83 models like DART-FT spend much time and memory tracking fluxes that contribute little to  
84 the simulated images. Based on the Bidirectional Path Tracing (BDPT) algorithm (Veach,  
85 1998), based on Monte Carlo modelling, the new DART mode called DART-Lux (Wang et al.,  
86 2022) highly reduces computer time and memory requirements to simulate images of large and  
87 complex landscapes. Therefore, we designed a novel SIF modelling method adapted to the  
88 BDPT algorithm for accurate and computationally efficient simulations of SIF RS images of  
89 3D vegetation canopies. To our knowledge, no similar SIF modelling method has ever been  
90 developed for BDPT algorithms.

#### 91 **II. DART-Lux**

92 DART is an accurate and comprehensive 3D RT model developed at CESBIO since 1992  
93 and patented in 2003. It simulates RS images of VIS / NIR / TIR spectro-radiometers, LiDAR



94 observations, and 3D RB of natural and urban landscapes (Wang et al., 2020). Its standard  
 95 mode, DART-FT, represents landscapes by 3D arrays of voxels filled with facets (*e.g.*,  
 96 vegetation, buildings), turbid medium and fluids. It iteratively tracks radiation in a user-defined  
 97 number of discrete directions. DART-Lux, DART's latest mode (Wang et al., 2022), uses the  
 98 BDPT algorithm with Monte Carlo integration techniques. It can largely decrease time and  
 99 memory requirements for DART images simulation of large and complex landscapes. It uses  
 100 the geometry instance, “depth-first” approaches (Cormen et al., 2009) and the BDPT algorithm  
 101 (Pharr et al., 2016) that preferentially tracks fluxes that contribute most to observations by  
 102 constructing paths that start both from the sensor and light sources. It is adapted to any  
 103 configuration with any light sources and landscape elements with any Bidirectional Scattering  
 104 Distribution Function (BSDF). The radiance measurement  $L^{(j)}$  of pixel  $j$  of the simulated  
 105 image is:

$$L^{(j)} = \int_{\mathcal{D}} C^{(j)}(\bar{p}) dA(\bar{p}) \quad (1)$$

106 where  $\bar{p}$  is a light transport path,

107  $\mathcal{D}$  is the set of all light transport paths.  $\mathcal{D} = \bigcup_{k=1}^{\infty} \mathcal{D}_k$ , with  $\mathcal{D}_k$  the set of all paths  
 108  $\bar{p}_k = (p_0, \dots, p_k)$  of length  $k$  (*i.e.*,  $k$  segments,  $k+1$  vertices  $p_i$ ;  $i \in [0, k]$ ,  $p_0$  on the sensor,  $p_k$   
 109 on the light source),

110  $dA(\bar{p})$  is the area product for path  $\bar{p}$ ; *e.g.*,  $dA(\bar{p}_k) = dA(p_0) \dots dA(p_k)$  with area  $dA(p_i)$  at  
 111 vertex  $i$

112 and  $C^{(j)}(\bar{p})$  is the contribution function of path  $\bar{p}$  to the measurement  $L^{(j)}$  of pixel  $j$ .

113  $L^{(j)}$  is computed as:

$$L^{(j)} = \int_{A_0} \int_{\Omega_0} W_e^{(j)}(p_0, \Omega) \cdot L(p_1 \rightarrow p_0) \cdot |\cos \theta_i^{p_0}| \cdot d\Omega dA(p_0) \quad (2)$$

114 where  $A_0$  is lens area,

115  $\Omega_0$  is the solid angle that encloses all incident directions from the optical system to the sensor  
 116 plane,

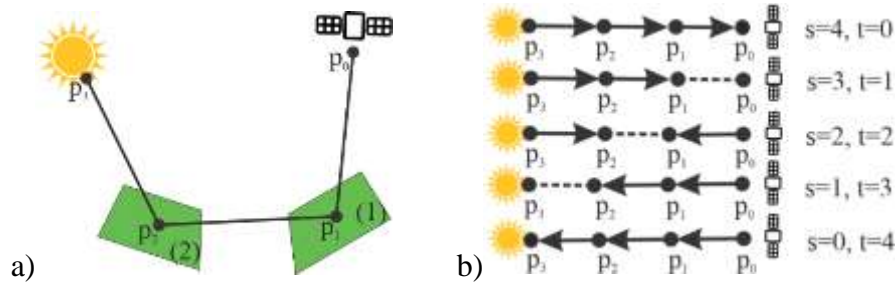
117  $W_e^{(j)}(p_0, \Omega)$  is the importance function (Nicodemus, 1978),

118  $\theta_i^{p_0}$  is the angle between the incident direction and the sensor principal optical axis

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119 and  $L(p_1 \rightarrow p_0) = \sum_{k=1}^{\infty} L(\bar{p}_k)$  is the radiance at sensor's vertex  $p_0$  from a surface's vertex  $p_1$   
 120 with  $L(\bar{p}_k)$  the radiance incident on  $p_0$  due to all paths  $\bar{p}_k$  of length  $k$ ; *e.g.*,  $\bar{p}_k =$   
 121  $(p_k, \dots, p_1, p_0)$ .

122 The radiance incident at vertex  $p_i$  of a path  $\bar{p}_k$  is the radiance from the vertex  $p_{i+1}$  that  
 123 illuminates the vertex  $p_i$ . A path results of the connection of a vertex of the sensor sub-path  
 124 created with  $t$  vertices from the sensor and a vertex of the source sub-path created with  $s$   
 125 vertices from the light source. Figure 1 shows a case with four vertices ( $p_0, p_1, p_2, p_3$ ), with  $p_0$   
 126 on the sensor and  $p_3$  on the source. In DART-Lux, the maximum scattering order (*i.e.*, number  
 127 of ray bounces on the scene surfaces) is a user-defined parameter. It defines the maximum  
 128 length of the light transport paths. In this figure, this maximum length is three ( $k = 3$ : 4  
 129 vertices and 3 segments) and the scattering order is 2.



130 a) Path  $\bar{p}_3$  with four vertices  $p_i$  ( $i \in \{0..k\}$  with  $k = 3$ ). b) The five ways to  
 131 construct  $\bar{p}_3$ , with  $s$  and  $t$  vertices ( $s+t = k+1 = 4$ ) for the sources and sensor sub-  
 132 paths, respectively.  
 133

134 In DART-Lux, the BDPT algorithm estimates  $L^{(j)}$  at sensor  $p_0$  from the contributions of  
 135 sampled paths constructed by incremental path tracing from both the light source and the sensor.  
 136 For example, if a path  $\bar{p}_k$  starts from the sensor, a point  $p_0$  is randomly sampled on the sensor  
 137 and a ray is traced from  $p_0$  and in the direction defined by sensor properties, until intersecting  
 138 a surface at a point  $p_1$ . Then, the path is iteratively constructed using the two steps:

- 139 1) At each vertex  $p_i$ , starting from  $i=1$ , sample a new direction according to the BSDF,  
 140 knowing the incident direction. Stop if  $i=k$ .
- 141 2) Find the next vertex  $p_{i+1}$  by tracing a ray from  $p_i$  along the sampled direction.

142 A Monte Carlo integration technique estimates the pixel radiance measurement with an  
 143 importance sampling technique (Kalos & Whitlock, 1986). Paths that most impact the radiance

144 reaching the sensor have a higher probability to be sampled. Multiple Importance Sampling  
 145 (MIS) (Veach & Guibas, 1995) is used to combine the different ways to sample the same path  
 146 (e.g., Figure 1.b shows the five ways to sample the path in Figure 1.a) using weighting functions  
 147 that give the weight  $w_i(x)$  per sample  $x$  drawn from the sampling way  $i$ . The Russian Roulette  
 148 (Veach & Guibas, 1995) is used to randomly stop the calculation at a certain path length to save  
 149 computer time. A probability  $q$  is set to stop a ray and not to evaluate the integrand for the  
 150 particular sample, and a probability  $(1-q)$  to evaluate the integrand and to weight it by  $\frac{1}{1-q}$ , to  
 151 account for all the samples that are not evaluated. The theory of DART-Lux was presented in  
 152 more details by Wang et al. (2022).

153 The DART-Lux image (5 m resolution, 100 bands in [0.4-0.85  $\mu\text{m}$ ]) of the  $3 \times 3 \text{ km}^2$   
 154 Ripperdan farm site with vines and more than 600.000 trees (Figure 12.b) shows its potential.  
 155 It needed 16.9 GB of memory and 13 min 4 s of simulation time with an Intel Xeon W-2295  
 156 CPU @ 3.00GHz (18 cores, 36 threads). DART-FT was not run because it needed about 50 TB  
 157 of memory and 1600 h of simulation time.

158

### 159 III. DART-Lux canopy SIF modelling

160 Despite its interest in accurate and fast radiance simulations of large landscapes, to our  
 161 knowledge, the BDPT algorithm has never been applied to canopy SIF modelling. Its adaptation  
 162 to SIF modelling in DART-Lux is presented here. It relies on the surface form of the Light  
 163 Transport Equation (LTE) to compute as an integral over all scene surfaces  $A$  the radiance  
 164 reaching a vertex  $p$  from a vertex  $p'$  (Figure 2):

$$L(p' \rightarrow p) = L_e(p' \rightarrow p) + \int_A f(p'' \rightarrow p' \rightarrow p) \cdot L(p'' \rightarrow p') \cdot G(p'' \leftrightarrow p') \cdot dA(p'') \quad (3)$$

165 where  $L_e(p' \rightarrow p)$  is the radiance emitted from  $p'$  to  $p$ , if  $p'$  belongs to a light source,  
 166  $L_e(p' \rightarrow p) = 0$  otherwise,

167  $G(p'' \leftrightarrow p') = V(p'' \leftrightarrow p') \cdot \frac{|\cos\theta_o''| \cdot |\cos\theta_i'|}{\|p' - p''\|^2}$ , with index  $o$  for outgoing and index  $i$  for  
 168 incident,

169  $f(p'' \rightarrow p' \rightarrow p)$  is the BSDF of surface  $\Sigma$ ,

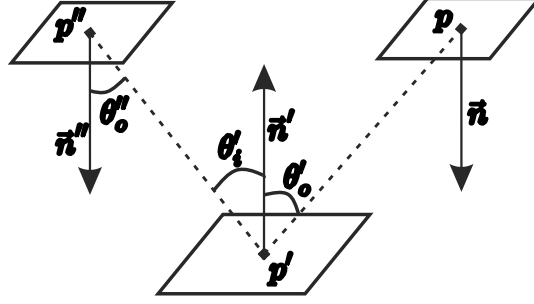
170  $L(p'' \rightarrow p')$  is the radiance reaching  $p'$  from  $p''$ ,

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171  $V$  is the binary visibility function:  $V(p'' \leftrightarrow p')=1$  if  $p'$  and  $p''$  are mutually visible, and 0  
 172 otherwise,

$$173 \quad \cos\theta_0'' = \vec{n}'' \cdot \frac{\overrightarrow{p''p'}}{\|p'-p''\|}, \text{ and } \cos\theta_0' = \frac{\overrightarrow{p'p''}}{\|p'-p''\|} \cdot \vec{n}',$$

174  $\vec{n}'$  and  $\vec{n}''$  are the normal vectors to the surface  $\Sigma$  at  $p'$  and to the surface  $A$  at  $p''$ , respectively.



175

176 Figure 2. LTE geometry: the vertex  $p'$  scatters the ray coming from the vertex  $p''$  towards the  
 177 vertex  $p$

178 Expanding Eq (3) by iteratively replacing  $L(p'' \rightarrow p')$  by its right-hand term gives  $L(\bar{p}_k)$  for  $k \geq$   
 179 2:

$$L(\bar{p}_k) = \int_A \int_A \dots \int_A L_e(p_k \rightarrow p_{k-1}) \cdot \left( \prod_{i=1}^{k-1} f(p_{i+1} \rightarrow p_i \rightarrow p_{i-1}) \cdot G(p_{i+1} \leftrightarrow p_i) \right) \cdot dA(p_2) \dots dA(p_k) \quad (4)$$

180 We denote  $P(\bar{p}_k)$  the integrand in Eq (4), and  $T(\bar{p}_k)$ , the “light path throughput”, the term  
 181 between brackets in  $P(\bar{p}_k)$ :

$$T(\bar{p}_k) = \prod_{i=1}^{k-1} f(p_{i+1} \rightarrow p_i \rightarrow p_{i-1}) \cdot G(p_{i+1} \leftrightarrow p_i) \quad (5)$$

$$P(\bar{p}_k) = L_e(p_k \rightarrow p_{k-1}) \cdot T(\bar{p}_k) \quad (6)$$

182 If  $p_i$  belongs to a bi-Lambertian surface, with normal  $\vec{n}_i$ , reflectance  $\rho_i$  and transmittance  $\tau_i$ :

$$f(p_{i+1} \rightarrow p_i \rightarrow p_{i-1}) = \begin{cases} \frac{\rho_i}{\pi}, & \text{if } (\overrightarrow{p_i p_{i+1}} \cdot \vec{n}_i) \cdot (\overrightarrow{p_i p_{i-1}} \cdot \vec{n}_i) \geq 0 \\ \frac{\tau_i}{\pi}, & \text{otherwise} \end{cases} \quad (7)$$

183 As for DART-FT (Malenovský et al., 2021), the Fluspect model (Vilfan et al., 2018) is used to  
 184 simulate leaf-level SIF. It uses the leaf biochemical properties and *fges* input parameters to  
 185 compute four leaf EEFMs (Excitation-Emission Fluorescence Matrices)  $M_{x,y,i,j}$  for the  $N$  user

186 defined spectral bands ( $i \in \{1..N\}$  for excitation and  $j \in \{1..N\}$  for emission), for the  
 187 photosystem  $x$  (PSI or PSII) and direction  $y$  (forward or backward). The reflectance  $\rho$  and  
 188 EEFM backward matrices ( $M_{x,backward,ij}$ ) play equivalent roles for scattering and SIF  
 189 emission respectively, and so do the surface transmittance  $\tau$  and EEFM forward matrices  
 190 ( $M_{x,forward,ij}$ ). In the Fluspect model, the leaves are bi-Lambertian and SIF emitted radiance  
 191 is isotropic. Therefore, the direction sampling method for SIF is the same as for scattering by  
 192 bi-Lambertian surfaces with the PDF  $p(\Omega) = \frac{\cos \theta}{\pi}$  where  $\theta$  is the angle between the surface  
 193 normal and the sampled direction  $\Omega$ , for any incident direction.

194 To estimate the pixel radiance measurement, the contribution of each sampled path is evaluated  
 195 by multiplying the integrand  $P(\bar{p}_k)$  of Eq (4) by the importance function and the cosine term  
 196 in Eq (2).

197 For  $N$  simulated spectral bands, the light source spectral radiance  $L_e$ , the bi-Lambertian surface  
 198 spectral reflectance and transmittance, and also the sub- and full-path throughputs are vectors  
 199 of  $N$  elements. A path throughput is computed by successive element wise vector  
 200 multiplications of the multi-spectral reflectance or transmittance value at each vertex by a  
 201 geometric term  $G$ , divided by  $\pi$  (Eq (5), (7)). This product is associative and can be computed  
 202 starting from the light source or starting from the sensor. A full path being the connection of a  
 203 light sub-path and a sensor sub-path, its throughput is the element wise product of the light and  
 204 sensor sub-path throughputs. Its multiplication by the light radiance  $L_e(p_k \rightarrow p_{k-1})$  gives the  
 205 integrand  $P(\bar{p}_k)$ .

206 For the simplicity of the equations below, we avoid writing the scalar multiplicative terms  $G$   
 207 and  $\frac{1}{\pi}$ . They are still considered in the computations. If the SIF emission is considered, three  
 208 components of the radiance need to be computed: 1) the total radiance including the scattered  
 209 radiation plus SIF emission, 2) the PSI SIF radiance component, 3) the PSII SIF radiance  
 210 component. For  $N$  simulated spectral bands, a fluorescent surface  $S_l$  is characterized by four  
 211  $N \times N$  EEFM, in addition to its non-fluorescent BSDF. For photosystem  $x$  and for direction  $y$ ,  
 212 the EEFM is:

213 
$$M_{xy}^l = \begin{pmatrix} f_{xy1,1}^l & \cdots & f_{xy1,N}^l \\ \vdots & \ddots & \vdots \\ f_{xyN,1}^l & \cdots & f_{xyN,N}^l \end{pmatrix}$$

### 3.1 VEGETATION SIMULATED AS FACETS

214 where  $f_{xyi,j}^l$  is the EEFM element for an excitation spectral band (central wavelength:  $\lambda_i$ ,  
215 bandwidth:  $\Delta\lambda_i$ ) and an emission band ( $\lambda_j, \Delta\lambda_j$ ),

216 For a path with two segments, the integrand of SIF radiance component of photosystem  $x$  and  
217 direction  $y$  is the matrix product of the light source spectral radiance  $L_e$  and the EEFM  $M_{xy}$ :

$$218 \quad P_x(\bar{p}_2) = L_e \times M_{xy}^l = (e_1, e_2, \dots, e_N) \times \begin{pmatrix} f_{xy1,1}^l & \dots & f_{xy1,N}^l \\ \vdots & \ddots & \vdots \\ f_{xyN,1}^l & \dots & f_{xyN,N}^l \end{pmatrix} = \left( \sum_{i=1}^N e_i \cdot f_{xyi,1}^l, \dots, \sum_{i=1}^N e_i \cdot f_{xyi,N}^l \right)$$

219 Therefore, for a path  $\bar{p}_k$  with  $k+1$  vertices  $p_l, l \in \{0..k\}$ , the integrand for the total radiance  
220 (*i.e.*, sum of scattered radiance, PSI and PSII SIF emissions radiance) is:

$$P_{total}(\bar{p}_k) = L_e \times T_{tot}(\bar{p}_k) \quad (8)$$

221 where  $T_{tot}(\bar{p}_k) = T_{tot}^1 \times \dots \times T_{tot}^{k-1}$  is the total throughput,

$$222 \quad T_{tot}^l = R_l + M_{PSIy}^l + M_{PSIIy}^l = \begin{pmatrix} r_1^l + f_{PSIy1,1}^l + f_{PSIIy1,1}^l & \dots & f_{PSIy1,N}^l + f_{PSIIy1,N}^l \\ \vdots & \ddots & \vdots \\ f_{PSIyN,1}^l + f_{PSIIyN,1}^l & \dots & r_N^l + f_{PSIyN,N}^l + f_{PSIIyN,N}^l \end{pmatrix},$$

223  $r_i^l$  is the reflectance or transmittance of the surface  $S_l$  at the band ( $\lambda_i, \Delta\lambda_i$ ),  $R_l = \begin{pmatrix} r_1^l & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & r_N^l \end{pmatrix}$ ,

224 and  $f_{PSIy,i,j}^l$  and  $f_{PSIIy,i,j}^l$  the EEFM elements for an excitation band ( $\lambda_i, \Delta\lambda_i$ ) and an emission  
225 band ( $\lambda_j, \Delta\lambda_j$ ) for PSI and PSII respectively, for direction  $y$ .

226 As the matrix product is associative, the product in Eq (8) can be cut into a light sub-path sub-  
227 product (*i.e.*,  $N$ -element vector resulting from successive vector-matrix products), and a sensor  
228 sub-path sub-product (*i.e.*,  $N \times N$  matrix resulting from successive matrix-matrix products).

229 However, Eq (8) provides only the total radiance ( $N$ -element vector). To have the PSI and PSII  
230 radiance separately as well, two additional  $N$ -element vectors need to be computed. For the  
231 path  $\bar{p}_k$ , in addition to  $P_{total}(\bar{p}_k)$ , the  $P_{PSI}(\bar{p}_k)$  and  $P_{PSII}(\bar{p}_k)$  need to be computed. For a light  
232 path  $\bar{p}_3$  with 3 segments (two fluorescent surfaces) (Figure 1),  $P_{PSI}(\bar{p}_3)$  and  $P_{PSII}(\bar{p}_3)$  are:

$$P_{PSI}(\bar{p}_3) = L_e \times [T_{tot}^1 \times M_{PSIy}^2 + M_{PSIy}^1 \times R_2] \quad (9)$$

$$P_{PSII}(\bar{p}_3) = L_e \times [T_{tot}^1 \times M_{PSIIy}^2 + M_{PSIIy}^1 \times R_2] \quad (10)$$

233 The bracketed terms in Eq (9) and (10) represent the interactions between the two surfaces that  
 234 generate the two SIF radiance components. Eq (9) and (10) cannot be written as an associative  
 235 product of terms each of which depends on the properties of a single vertex. Thus, they cannot  
 236 be computed starting both from the light source and from the sensor. Therefore, the block matrix  
 237  $M_B^l$  is introduced:

$$M_B^l = \begin{pmatrix} T_{\text{tot}}^l & M_{PSIy}^l & M_{PSIIy}^l \\ 0 & R_l & 0 \\ 0 & 0 & R_l \end{pmatrix} \quad (11)$$

238 The light radiance vector is also written as a block matrix:  $L_{e,B} = (L_{e,\text{total}}; L_{e,PSI}; L_{e,PSII})$ ,  
 239 where  $L_{e,\text{total}}$ ,  $L_{e,PSI}$  and  $L_{e,PSII}$  are  $N$ -element vectors. Since light sources do not emit SIF,  
 240  $L_{e,PSI}$  and  $L_{e,PSII}$  are null vectors. If  $M_B^{k-1}$  is the block matrix of the first surface hit by the light  
 241 source, the incident radiance vector  $L_{B,k-2} = L_{e,B} \times M_B^{k-1}$  at vertex  $k-2$  is:

$$L_{B,k-2} = (L_{e,\text{total}}; 0; 0) \times \begin{pmatrix} R_{k-1} + M_{PSIy}^{k-1} + M_{PSIIy}^{k-1} & M_{PSIy}^{k-1} & M_{PSIIy}^{k-1} \\ 0 & R_{k-1} & 0 \\ 0 & 0 & R_{k-1} \end{pmatrix} \quad (12)$$

$$\begin{aligned}
 242 \quad &= (L_{e,\text{total}} \times (R_{k-1} + M_{PSIy}^{k-1} + M_{PSIIy}^{k-1}); L_{e,\text{total}} \times M_{PSIy}^{k-1}; L_{e,\text{total}} \times M_{PSIIy}^{k-1}) \\
 243 \quad &= (L_{\text{total},k-2}; L_{PSI,k-2}; L_{PSII,k-2})
 \end{aligned}$$

244 Similarly, at vertex  $k-3$ , the incident radiance vector  $L_{B,k-3} = L_{B,k-2} \times M_B^{k-2}$  is:

$$L_{B,k-3} = (L_{\text{total},k-2}; L_{PSI,k-2}; L_{PSII,k-2}) \times \begin{pmatrix} R_{k-2} + M_{PSIy}^{k-2} + M_{PSIIy}^{k-2} & M_{PSIy}^{k-2} & M_{PSIIy}^{k-2} \\ 0 & R_{k-2} & 0 \\ 0 & 0 & R_{k-2} \end{pmatrix}$$

$$\begin{aligned}
 246 \quad &= (L_{\text{total},k-2} \times (R_{k-2} + M_{PSIy}^{k-2} + M_{PSIIy}^{k-2}); L_{\text{total},k-2} \times M_{PSIy}^{k-2} + L_{PSI,k-2} \times R_{k-2}; \\
 247 \quad &\quad L_{\text{total},k-2} \times M_{PSIIy}^{k-2} + L_{PSII,k-2} \times R_{k-2}) \\
 248 \quad &= (L_{\text{Total},k-3}; L_{PSI,k-3}; L_{PSII,k-3})
 \end{aligned}$$

249 And so on, for each vertex  $p_l$  of the light sub path until reaching the sensor, the exiting radiance  
 250 block matrix is:

$$L_{B,l} \times M_{B,l} = (L_{\text{total},l}; L_{PSI,l}; L_{PSII,l}) \times \begin{pmatrix} R_l + M_{PSIy}^l + M_{PSIIy}^l & M_{PSIy}^l & M_{PSIIy}^l \\ 0 & R_l & 0 \\ 0 & 0 & R_l \end{pmatrix}$$

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$$252 \quad = (L_{total,l} \times (R_l + M_{PSIy}^l + M_{PSIIy}^l); L_{total,l} \times M_{PSIy}^l + L_{PSI,l} \times R_l; L_{total,l} \times M_{PSII}^l + L_{PSII} \times R_l)$$

253 All components of the total, PSI and PSII spectral radiance terms of  $p_l$  are considered:

254 -Total radiance  $L_{total,l} \times (R_l + M_{PSIy}^l + M_{PSIIy}^l)$  of surface  $p_l$  hit by a ray of incident radiance  
255  $L_{total,l}$

256 -PSI radiance: sum of the emitted PSI radiance  $L_{total,l} \times M_{PSIy}^l$  at  $p_l$  due to  $L_{total,l}$ , and PSI  
257 radiance  $L_{PSI,l} \times R_l$  coming from the previous vertex and scattered at  $p_l$ .

258 -PSII radiance: sum of the emitted PSII radiance  $L_{total,l} \times M_{PSII}^l$  at  $p_l$  due to  $L_{total,l}$ , and PSII  
259 radiance  $L_{PSII,l} \times R_l$  coming from the previous vertex and scattered at  $p_l$ .

260 These equations can be used starting from the light source and starting from the sensor because  
261 they include associative products of matrices and each matrix depends on the properties of a  
262 single vertex. For a light path with  $L + 2$  vertices (*i.e.*,  $L$  hit surfaces of matrices  $M_B^l$  with  $l \in$   
263  $\{1..L\}$ ), the integrand  $P_B(\bar{p}_{L+2})$  including the total, PSI and PSII signals from this path is:

$$264 \quad P_B(\bar{p}_{L+2}) = L_{e,B} \times M_{B,1} \times M_{B,2} \times \dots \times M_{B,L}$$

265 If the light path  $\bar{p}_{L+2}$  has  $S$  vertices in the light sub-path and  $T$  vertices in the sensor sub-path,  
266 excluding the light source and sensor vertices ( $L+2=S+T$ ), the throughput of the light sub-  
267 path is  $M_B^{light} = M_{B,1} \times M_{B,2} \times \dots \times M_{B,S}$  and of the sensor sub path  
268  $M_B^{sensor} = M_{B,S+1} \times M_{B,S+2} \times \dots \times M_{B,S+T}$ . After connecting the two sub-paths, the integrand is:

$$P_B(\bar{p}_{L+2}) = L_{e,B} \times M_B^{light} \times M_B^{sensor} \quad (13)$$

269 The light sub-path starts from the light source, then hits the surfaces from 1 to  $S$ . It gives the  
270 block matrix  $E_B \times M_B^{light}$  of three  $N$ -element vectors. The sensor sub-path hits the surfaces  $S+T$   
271 to  $S+1$ . The matrix product being not commutative,  $E_B \times M_B^{light}$  and  $M_B^{sensor}$  are computed in  
272 opposite directions.

273 Eq (13) is computationally expensive. For  $N$  spectral bands, a sensor sub-path throughput is  
274 a  $3N \times 3N$  matrix. For optimization, diagonal matrices are considered whenever possible when  
275 multiplying matrices, and only  $R_l + M_{PSIy}^l + M_{PSII}^l$ ,  $M_{PSI}^l$ ,  $M_{PSII}^l$  and  $R_l$  only are stored instead of



276  $M_B^l = \begin{pmatrix} R_l + M_{PSI}^l + M_{PSII}^l & M_{PSI}^l & M_{PSII}^l \\ 0 & R & 0 \\ 0 & 0 & R \end{pmatrix}$  because the product of matrices of this form has the  
 277 same form (*cf.* Appendix 1).

278 As DART-FT (Malenovský et al., 2021), DART-Lux can import SCOPE  $\eta$  factors vertical  
 279 profiles for sunlit and shaded leaves to account for the influence of local bioclimatology on  
 280 leaf-level SIF emission. With the hypothesis that only PSII emission is affected, we have:

$$281 \quad M_{B,\eta} = \begin{pmatrix} R + M_{PSI} + \eta \cdot M_{PSII} & M_{PSI} & \eta \cdot M_{PSII} \\ 0 & R & 0 \\ 0 & 0 & R \end{pmatrix}$$

282 Increasing the number of Monte Carlo samples/pixel  $N_{\text{samples}}$  in the simulated images improves  
 283 accuracy and increases simulation time. The optimal average  $N_{\text{samples}}$  depends on the scene  
 284 properties, pixel size, and expected precision and simulation time.

285 PSI and PSII radiance images (Figure 12) of the  $3 \times 3 \text{ km}^2$  Ripperdan zone illustrate the  
 286 potential of DART-Lux SIF modelling for large landscapes. It needed 42.9 GB of memory and  
 287 2h 44 min in simulation time with an Intel Xeon W-2295 CPU @ 3.00GHz (18 cores, 36  
 288 threads). DART-FT was not run due to huge computational demands: more than 100 TB of  
 289 memory and 15000 h of simulation time.

#### 290 IV. Assessment of DART-Lux SIF modelling

291 Malenovský et al. (2021) validated DART-FT SIF modelling against the SCOPE/mSCOPE  
 292 model for homogeneous canopies. Here, the accuracy and computer efficiency of DART-Lux  
 293 SIF modelling are assessed for three canopies, using DART-FT SIF as a reference. DART-Lux  
 294 is also compared to SCOPE for homogeneous scenes. These model cross-comparisons between  
 295 models  $M_1$  and  $M_2$  for  $N$  spectral bands and a given physical quantity  $q$ , are done with the  
 296 Mean Absolute Relative Difference (MARD):

$$297 \quad \text{MARD}_{M_1/M_2} = \frac{1}{\sum_{i=1}^N \Delta\lambda_i} \sum_{i=1}^N \frac{|q_{M1,i} - q_{M2,i}|}{q_{M2,i}} \cdot \Delta\lambda_i \quad (14)$$

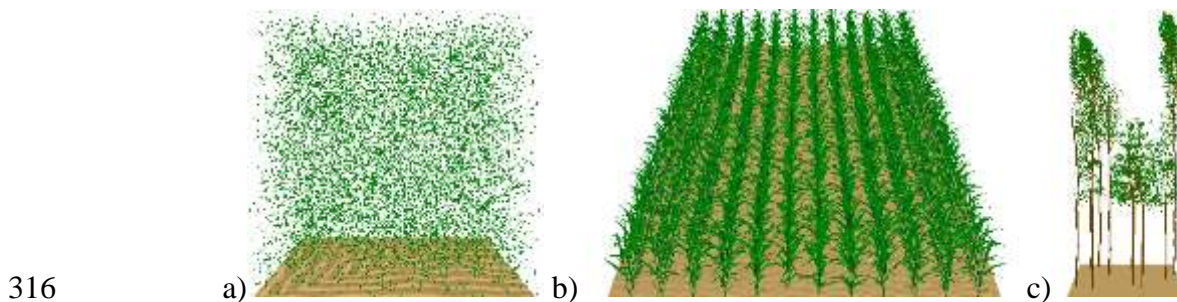
#### 298 IV.1 Study cases

299 Three vegetation canopies (Figure 3) are studied. 1) Homogeneous turbid scene: 1 m high,  
 300 LAI=1, spherical LAD, nadir observation and solar direction ( $\theta_s=30^\circ$ ,  $\phi_s=225^\circ$ ). 2) Maize crop

### 3.1 VEGETATION SIMULATED AS FACETS

301 field: 7.5 m  $\times$  5 m scene, 600 maize plants, 40 cm spaced rows, 15 cm within row plant  
302 distance, LAI=1.9, three viewing directions (nadir;  $\theta_v=30^\circ, \phi_v=0^\circ$ ;  $\theta_v=60^\circ, \phi_v=0^\circ$ ), and  
303 three solar directions ( $\theta_s=42.78^\circ, \phi_s=82.98^\circ$ ;  $\theta_s=31.46^\circ, \phi_s=69.88^\circ$ ;  
304  $\theta_s=21.41^\circ, \phi_s=48.32^\circ$ ). 3) Tree plot: 10m x 10m scene, 10 randomly distributed trees  
305 "*populus\_tremuloides*" with branch and trunk reflectance from the DART spectral database,  
306 LAI=1.9, nadir viewing direction and ( $\theta_s=30^\circ, \phi_s=225^\circ$ ). Simulations are over [400-850 nm]  
307 with 451 bands ( $\Delta\lambda = 1$  nm) for the homogeneous site and maize field, and 45 bands ( $\Delta\lambda =$   
308 10 nm) for the tree plot. Atmosphere (gas model: USSTD76, aerosol model: RURALV23), leaf  
309 biochemistry and structure (Table 1), and ground reflectance "*loam\_gravelly\_brown\_dark*" in  
310 DART database. Spatial resolution is 0.1 m for the tree plot and the homogenous site. It is 0.5  
311 m and 0.01 m for the maize field, with 0.01 m selected to mimick the simulation of images of  
312 large scenes. It implied using fewer spectral bands in order to maintain reasonable  
313 computational needs for DART-FT: 35 excitation bands over [400-750 nm] and one emission  
314 band ( $\lambda_c = 765$  nm,  $\Delta\lambda = 1$  nm).

315



316

317 Figure 3. The simulated 3D mock-ups. a) Homogeneous medium b) Maize field. c) Tree plot.

318

319

Table 1. Leaf biochemistry and structure for the three study sites.

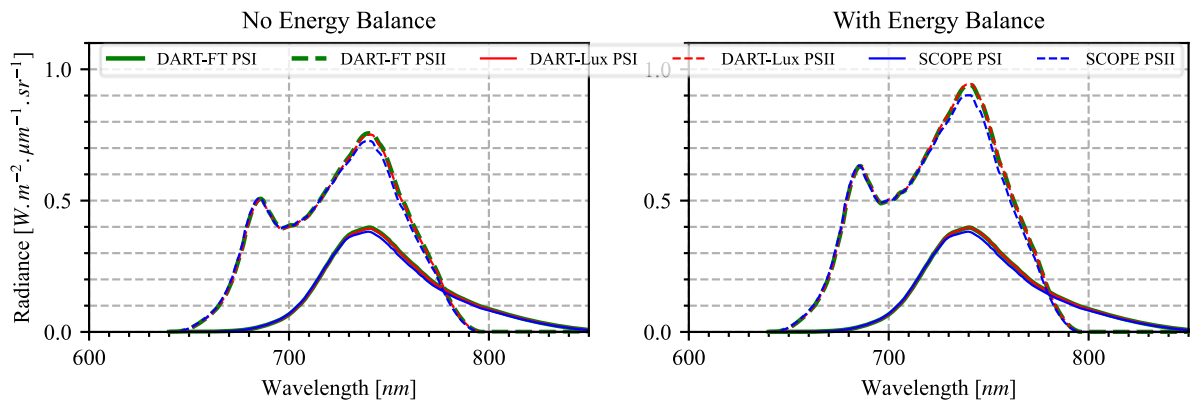
Parameter	Symbol	Unit	Homogeneous canopy	Maize field	Tree plot
Leaf structure parameter	$N$	-	1.8	1.5	1.8
Chlorophyll a+b content	$C_{ab}$	$\mu g. cm^{-2}$	45	50	30
Carotenoid content	$C_{ca}$	$\mu g. cm^{-2}$	15	15	10
Water content	$C_w$	$cm$	0.009	0.009	0.012
Dry matter content	$C_{dm}$	$g. cm^{-2}$	0.002	0.0021	0.01
$fqe$ for photosystem I	$\phi_{PSI}$	-	0.002	0.002	0.002
$fqe$ for photosystem II	$\phi_{PSII}$	-	0.01	0.01	0.01

320

321 **IV.2 Homogeneous turbid canopy**

322 SCOPE is a reference model for simulating the SIF radiance of homogeneous vegetation. Here,  
 323 DART-FT and DART-Lux SIF simulate the homogeneous turbid scene of SCOPE as a  
 324 homogeneous quasi turbid medium for two cases depending if SCOPE simulates or not the  
 325 energy balance (EB):

- 326 - No EB: the  $\eta$  factors are set to one in DART-FT and DART-Lux.
- 327 - EB: DART-FT and DART-Lux use the SCOPE  $\eta$  factors for the default meteorological
- 328 parameters.



329

330 Figure 4. Homogeneous site: DART-FT, DART-Lux and SCOPE PSI and PSII nadir radiance,  
 331 without (left) and with (right) computation of the canopy energy balance.

### 3.1 VEGETATION SIMULATED AS FACETS

332 Figure 4 shows DART-Lux, DART-FT and SCOPE PSI and PSII nadir radiance. DART-Lux  
333 closely matches DART-FT and, to a lesser extent, SCOPE. Without EB,  
334  $MARD_{\text{DART-Lux/DART-FT}}$  is 0.7% for PSI and 0.53% for PSII, and  $MARD_{\text{DART-Lux/SCOPE}}$  is  
335 5.24% for PSI and 4.93% for PSII. Without neglect of EB,  $MARD_{\text{DART-Lux/DART-FT}}$  is 0.08% for  
336 PSI and 0.19% for PSII, and  $MARD_{\text{DART-Lux/SCOPE}}$  is 5.57% for PSI and 5.15% for PSII.

#### 337 **IV.3 Maize field**

338 The canopy nadir reflectance (Figure 5) and SIF PSI and PSII radiance (Figure 6, Table 2)  
339 simulated by DART-FT, DART-Lux and SCOPE for the three viewing directions and three sun  
340 directions show that:

- 341 - DART-Lux and DART-FT match:  $MARD_{\text{reflectance}} < 1.3\%$  and  $MARD_{\text{SIF radiance}} < 1\%$ .
- 342 - DART-Lux and DART-FT poorly match SCOPE:  $MARD_{\text{reflectance}}$  up to 16% and  $MARD_{\text{SIF}}$   
343 radiance from 3% to 19%, depending on the solar and viewing angles, with larger MARD for  
344 large angles.

345 Table 3 shows the computer time and RAM needs of DART-Lux and DART-FT at 0.5 m and  
346 0.01 m resolutions, and also the main input parameters that influence their computational needs.  
347 Compared to DART-FT (200 discrete directions and illumination step =  $10^{-3}$  m), DART-Lux  
348 ( $7^2$  scene repetitions, maximal scattering order = 15, Russian Roulette starts at order 12 with  
349 cut-off probability = 0.5) decreases the memory by a factor of  $\approx 34$  and computer time by  $\approx 1.4$   
350 at 0.5 m resolution. It decreases the memory by  $\approx 48$  and computer time by  $\approx 50$  at 0.01 m  
351 resolution. Figure 7 shows nadir radiance images at 0.01 m resolution: DART-Lux RGB color  
352 composite, and also DART-Lux and DART-FT PSI and PSII nadir radiance images.

353 Table 2. Maize field: MARD of DART-Lux canopy SIF PSI and PSII radiance compared to  
 354 DART-FT and SCOPE for 3 viewing directions and 3 sun directions.

	Nadir	$\theta_v = 30^\circ \phi_v = 0^\circ$	$\theta_v = 60^\circ \phi_v = 0^\circ$
$\theta_s = 42.78^\circ$ $\phi_s = 82.98^\circ$	MARD <sub>DART-Lux/DART-FT</sub> :		
	PSI: 0.46%,	PSI: 0.56%,	PSI: 0.67%,
	PSII: 0.44%	PSII: 0.42%	PSII: 0.58%
	MARD <sub>DART-Lux/SCOPE</sub> :		
	PSI: 3.19%,	PSI: 9.61%,	PSI: 18.84%,
	PSII: 4.24%	PSII: 7.81%	PSII: 14.51%
$\theta_s = 31.46^\circ$ $\phi_s = 69.88^\circ$	MARD <sub>DART-Lux/DART-FT</sub> :		
	PSI: 0.53%,	PSI: 0.76%,	PSI: 0.71%,
	PSII: 0.43%	PSII: 0.61%	PSII: 0.40%
	MARD <sub>DART-Lux/SCOPE</sub> :		
	PSI: 4.04%,	PSI: 10.04%,	PSI: 16.78%,
	PSII: 4.30%	PSII: 8.03%	PSII: 12.87%
$\theta_s = 21.41^\circ$ $\phi_s = 48.32^\circ$	MARD <sub>DART-Lux/DART-FT</sub> :		
	PSI: 0.88%,	PSI: 0.92%,	PSI: 0.29%,
	PSII: 0.63%	PSII: 0.67%	PSII: 0.27%
	MARD <sub>DART-Lux/DART-FT</sub> :		
	PSI: 3.20%,	PSI: 9.05%,	PSI: 15.54%,
	PSII: 4.06%	PSII: 7.77%	PSII: 11.67%

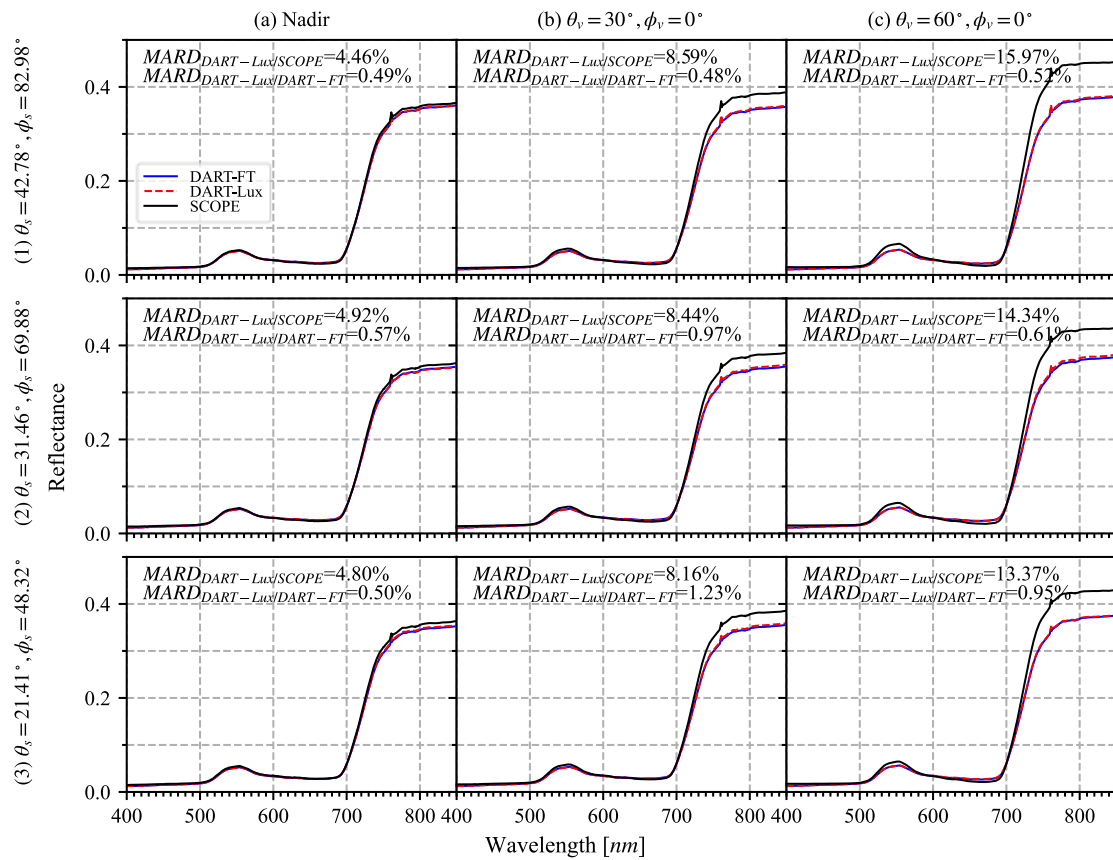
355

### 3.1 VEGETATION SIMULATED AS FACETS

356 Table 3. Maize field: input parameters and computational needs of DART-FT and DART-  
357 Lux.

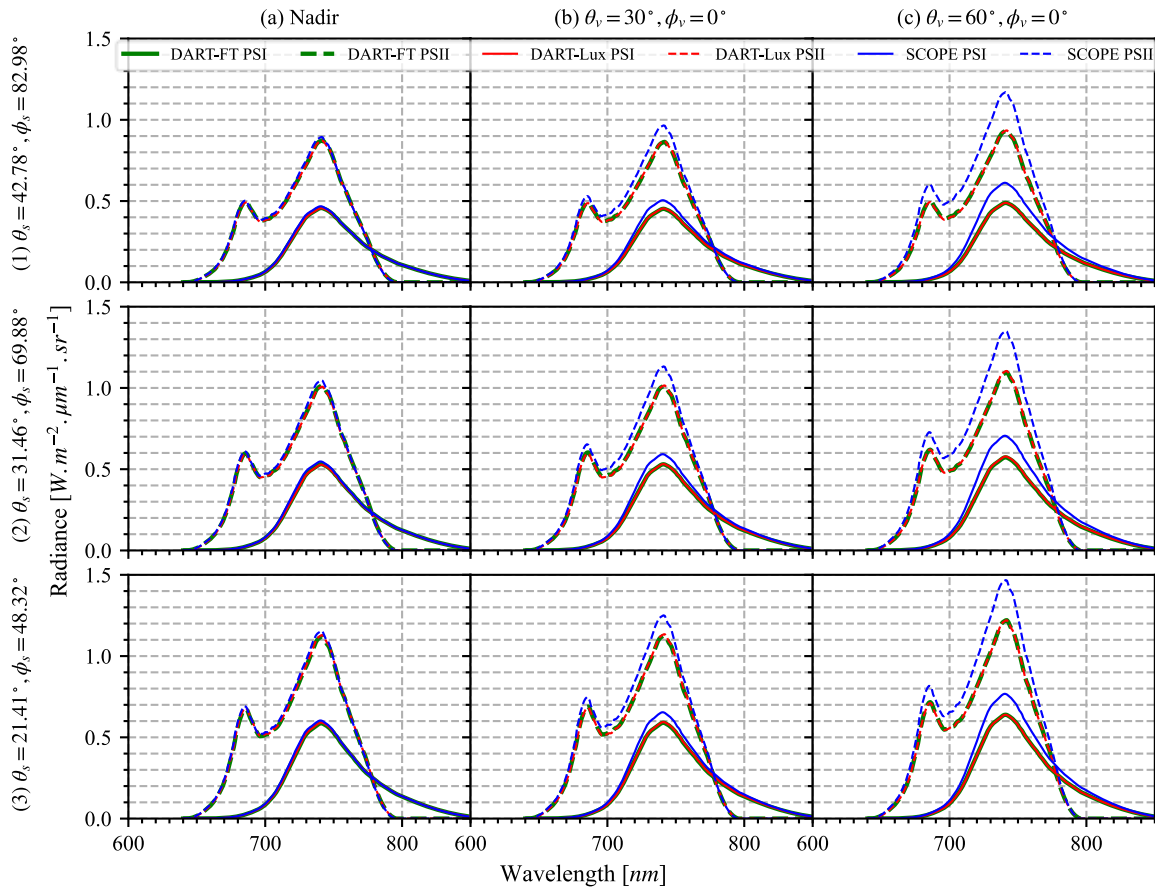
		DART-FT	DART-Lux		
5 m spatial resolution, 451 spectral bands	Viewing direction	All	Nadir	$\theta_v=30^\circ, \phi_v=0^\circ$	$\theta_v=60^\circ, \phi_v=0^\circ$
	Computer time	1 h 31 min	1 h 7 min	1 h 9 min	1 h 2 min
	Samples per pixel	-	100	120	180
	Memory	51 GB	1.5 GB		
0.01 m spatial resolution, 36 spectral bands	Viewing direction	All	Nadir		
	Computer time	8 h 13 min	10 min 10 s		
	Samples per pixel	-	20		
	Memory	105.8 GB	8.2 GB		

358



359

360 Figure 5. Maize field: DART-FT, DART-Lux and SCOPE reflectance for 3 solar directions and  
361 3 viewing directions with no account of bioclimatology on SIF emission.

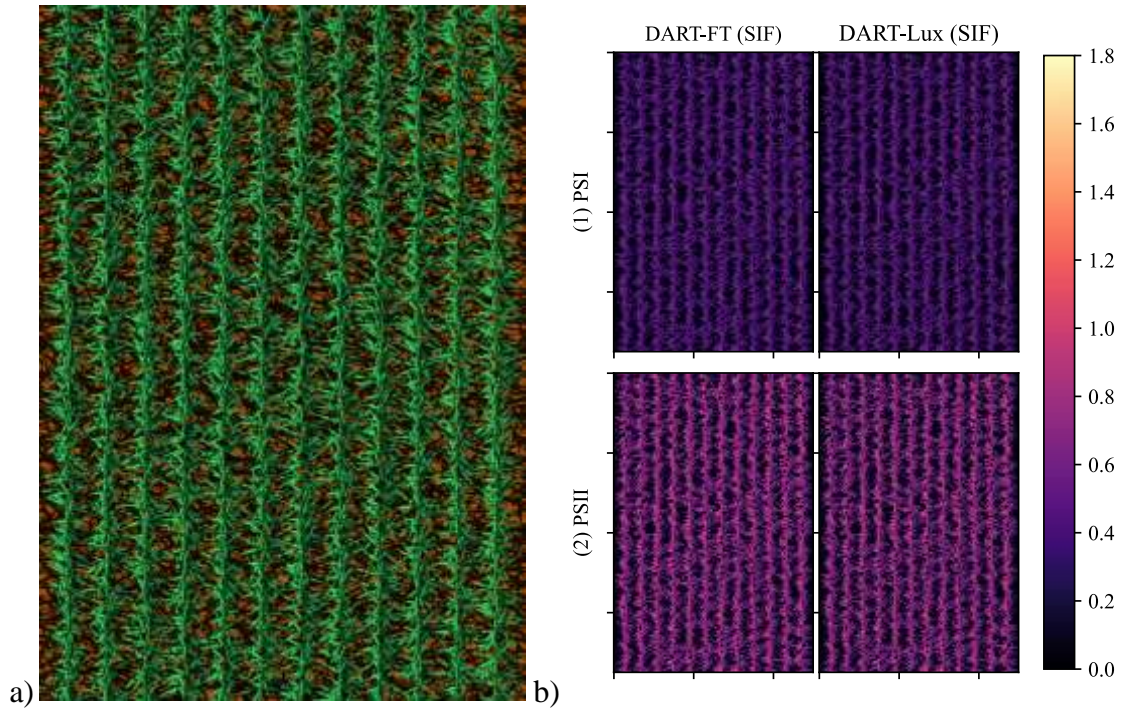


362

363 Figure 6: Maize field: DART-FT, DART-Lux and SCOPE SIF PSII and PSII radiance, for 3  
 364 solar directions and 3 viewing directions with no account of bioclimatology on SIF  
 365 emission.

366 DART-FT and DART-Lux were also run using the  $\eta$  factors calculated by SCOPE with its  
 367 default meteorological input parameters. Although these  $\eta$  factors should depend on the canopy  
 368 3D architecture, we made this approximation (*i.e.*, application of 1D information in a 3D model)  
 369 because of the unavailability of 3D energy balance model. DART-Lux and DART-FT match as  
 370 for the case "No energy balance": the MARD for canopy SIF radiance and for canopy  
 371 reflectance (not shown here) keep the same order of magnitude. The differences with SCOPE  
 372 are also similar.

373

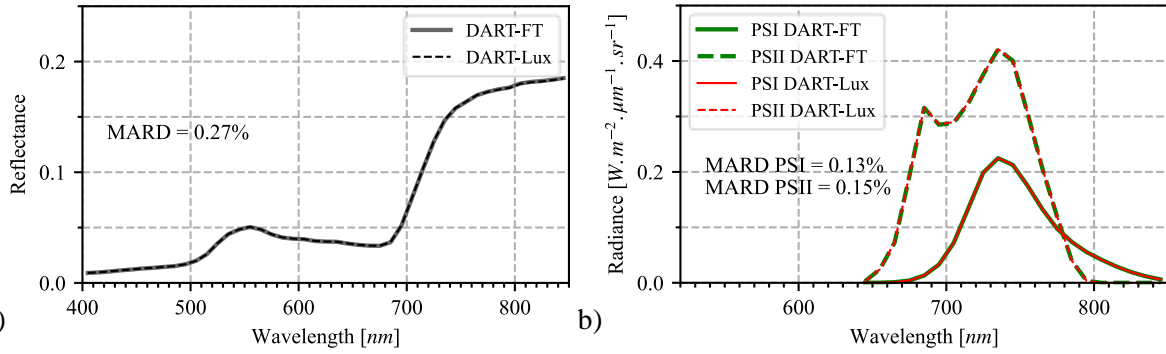


374 a) 375 Figure 7. Maize field: nadir radiance images at 1 cm resolution ( $\text{W}\cdot\text{m}^{-2}\cdot\mu\text{m}^{-1}\cdot\text{sr}^{-1}$ ). a) DART-  
 376 Lux RGB color composite. b) DART-FT and DART-Lux SIF (PSI and PSII).  
 377  $\lambda_c=765 \text{ nm}$ ,  $\Delta\lambda=1 \text{ nm}$ .

#### 378 IV.4 Trees plot simulation

379 The reflectance and SIF radiance of DART-Lux match DART-FT DART-FT (100 discrete  
 380 directions, illumination step =  $10^{-3} \text{ m}$ ), DART-Lux ( $17^2$  scene repetitions, maximal scattering  
 381 order = 15, Russian Roulette starts at order 12 with cut-off probability =0.5, 200 samples per  
 382 pixel) (Figure 8): MARD is 0.27% for reflectance and less than 0.15% for SIF radiance, with  
 383 memory need reduced by  $\sim 13$  and computer time by more than 5 times (Table 4). Figure 9  
 384 shows the root mean square deviation (RMSD) of DART-Lux and DART-FT PSI and PSII  
 385 radiance with the number of samples/pixel (*i.e.*, simulation time).





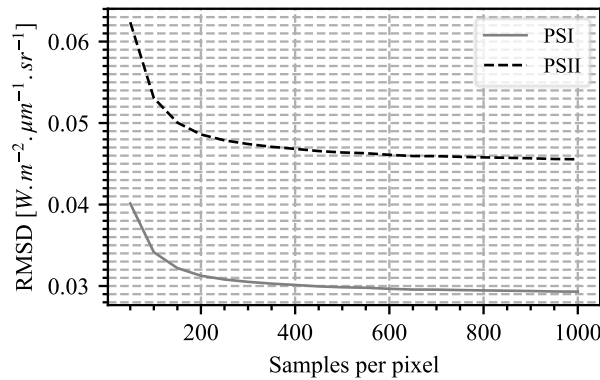
386

387 Figure 8. Tree plot: DART-Lux and DART-FT total (a) and PSI and PSII (b) nadir spectral  
388 radiance.

389 Table 4. Computational needs of DART-FT and DART-Lux for the tree plot simulation  
390 (spatial resolution: 0.1 m, 45 spectral bands)

	DART-FT	DART-Lux
Computer time	22 min	4 min
Memory	9.2 GB	0.715 GB

391



392

393 Figure 9. RMSD of the DART-Lux and DART-FT PSI and PSII radiance images at 765 nm as  
394 a function of the number of samples/pixel in DART-Lux.

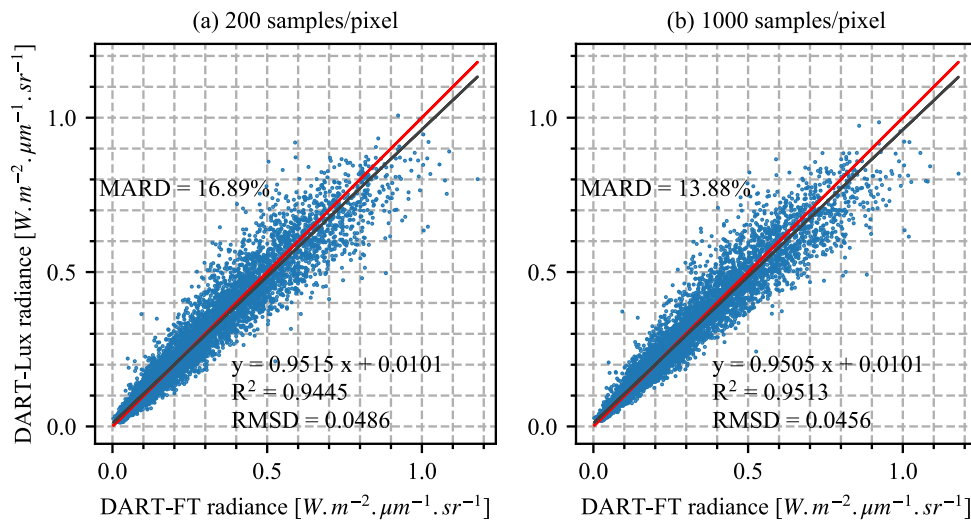
395 Figure 10 shows the pixel-wise comparison of DART-FT and DART-Lux PSII images at  
396 765 nm, for 200 samples/pixel and for 1000 samples/pixel. The pixel-wise MARD is computed  
397 by replacing the average on spectral bands by the average on the image pixels. The pixel-wise  
398 MARD for 200 samples/pixel (16.89%) is larger than for 1000 samples/pixel (13.88%).  
399 Inversely, the  $R^2$  slightly increases from 200 samples/pixel to 1000 samples/pixel. The MARDs  
400 are much higher than the spectrally averaged MARD for the total scene (0.15%, Figure 8) in

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401 particular because the images have many pixels. The MARDs and  $R^2$  for PSI (not shown here)  
 402 are nearly the same as for PSII.

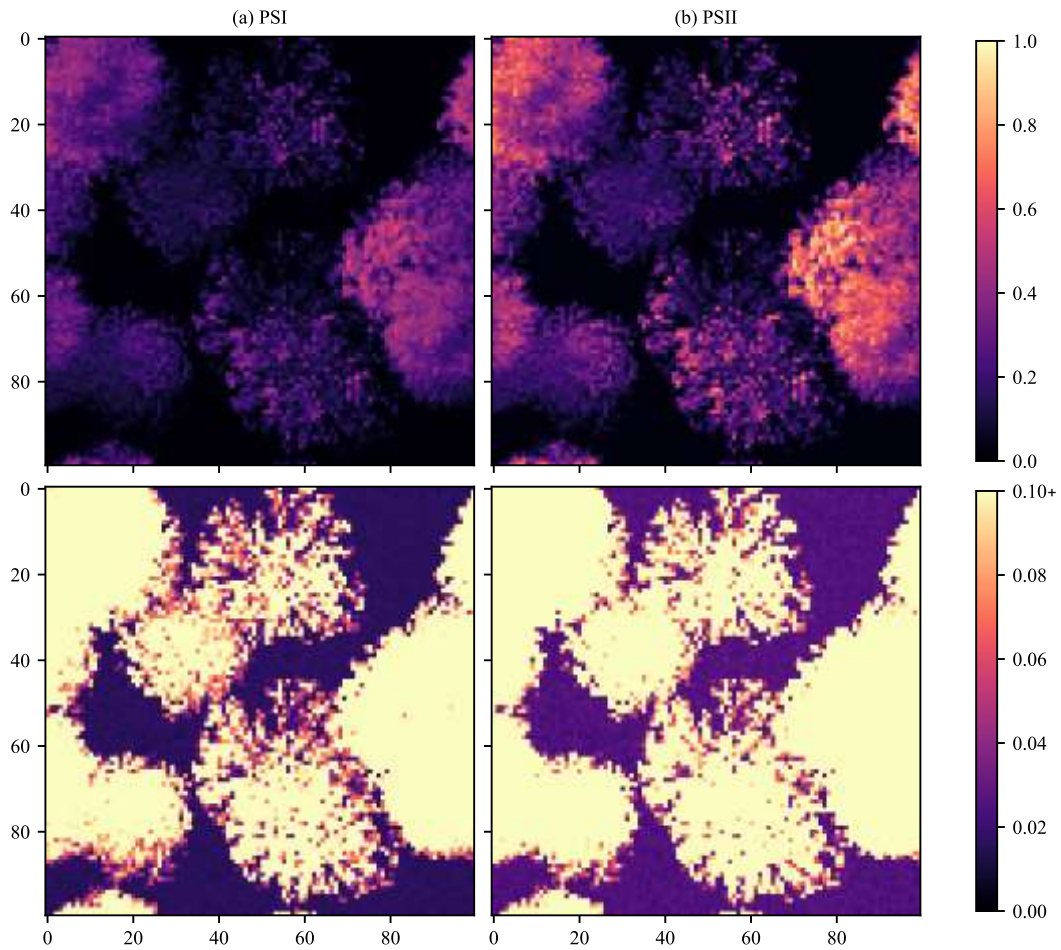
403 Figure 11 shows DART-Lux images of the tree plot with 1000 samples/pixel. The SIF signal  
 404 from the bare ground comes from the SIF radiation emitted by the vegetation that is scattered  
 405 by the ground.

406



407

408 Figure 10. Pixel-wise comparison of DART-FT and DART-Lux PSII radiance images with  
 409 samples/pixel = 200 (a) and 1000 (b).  $\theta_s=30^\circ$ ,  $\phi_s=225^\circ$ .  $\lambda_c = 765 \text{ nm}$ ,  $\Delta\lambda =$   
 410  $10 \text{ nm}$ .



411

412 Figure 11. Tree plot: DART-Lux PSI and PSII SIF nadir radiance images ( $\text{W}\cdot\text{m}^{-2}\cdot\mu\text{m}^{-1}\cdot\text{sr}^{-1}$ ),  
 413 with normal (top) and stretched (bottom) color scales.  $\lambda_c = 765 \text{ nm}$ ,  $\Delta\lambda = 10 \text{ nm}$ .

## 414 V. Discussion

415 DART-FT and DART-Lux have different radiative transfer modelling strategies. DART-FT  
 416 is determinist. It tracks radiation fluxes in  $N$  discrete directions that sub-divide the  $4\pi$  space  
 417 with an iterative approach that scatters at iteration  $i + 1$  radiation intercepted in iteration  $i$   
 418 (Gastellu-Etchegorry et al., 1996). DART-Lux is probabilistic. Indeed, it uses Monte-Carlo  
 419 integration techniques to solve the LTE by sampling the possible light paths, evaluating their  
 420 contributions, and giving higher importance weights to most likely paths (Wang et al., 2022).

421 For small scenes, DART-Lux and DART-FT SIF closely match, with relative difference  
 422 always smaller than 2%. This difference is small enough to be explained by the parameters that  
 423 drive the precision of DART-Lux (*e.g.*, number of samples/pixel) and DART-FT (*e.g.*,  
 424 dimension of voxels, numbers of discrete directions, etc.). For these scenes, compared to

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425 DART-FT, DART-Lux efficiency is not as pronounced as for larger sites as Ripperdan (Figure  
426 12).

427 Homogeneous vegetation: DART-Lux closely matches DART-FT and also SCOPE to a  
428 lesser extent. Its relative differences are less than 1% with DART-FT, and  $\approx 5\%$  for SCOPE.  
429 Four major factors can explain that differences are higher for SCOPE. 1) SCOPE simulates  
430 radiative transfer with four fluxes and assumes the isotropy of downward and upward scattered  
431 radiation, which is not exact (except for the special case of exactly horizontal leaves). On the  
432 other hand, DART-FT uses many (here: 200) discrete directions, which allows an accurate  
433 representation of the anisotropy of the downward and upward scattered radiation. DART-Lux  
434 simulates this anisotropy even more accurately than DART-FT because it can track photons in  
435 any direction. 2) SCOPE discretizes the LAD with 13 leaf zenith angles, whereas DART-FT  
436 and DART-Lux randomly sample the LAD with a number of samples equal to the number of  
437 facets used to simulate the quasi-turbid medium. DART and SCOPE more closely match  
438 (results not shown here) by introducing into the code of SCOPE a more accurate LAD with 90  
439 leaf zenith angles. 3) The quasi-turbid medium is not exactly the turbid medium of SCOPE  
440 because its facets cannot be infinitely small and infinitely numerous. 4) The application of the  
441 SCOPE  $\eta$  factors in SCOPE, on the one hand, and in DART-FT and DART-Lux, on the other  
442 hand, differs. Indeed, SCOPE applies vertical profiles of  $\eta$  factors to homogeneous layers and  
443 DART to facets with interpolations on the  $\eta$ . For this simulation, the  $\eta$  factors (*i.e.*, impact of  
444 local climatology) do not impact PSI SIF radiance and increase PSII radiance by  $\approx 25\%$ .

445 Maize field: the DART-FT and DART-Lux total and SIF radiance closely match and tend to  
446 be smaller than for SCOPE, especially for oblique viewing directions, with relative difference  
447 possibly larger than 25% for PSII in the NIR. This difference is explained by the canopy 3D  
448 architecture (3D maize plants, rows) with the clumping of the maize plants in DART, whereas  
449 for SCOPE, the vegetation is homogeneous which is more effective for intercepting radiation  
450 and therefore for SIF emission, and also for allowing the emitted SIF radiation to escape the  
451 canopy. The  $MARD_{\text{DART-SCOPE}}$  exceeds 10% in most configurations and increases to reaches  
452 18% for the oblique viewing angle  $\theta_v = 60^\circ$ . Indeed, in SCOPE simulations, radiation  
453 interception and therefore SIF emission occur mostly at the top layers of the canopy. When  $\theta_v$   
454 increases, the SIF seen by the sensor increases because the contribution of the top layers to the  
455 signal increases. Similarly, for the 3D maize scene, the SIF seen by the sensor from the plants

456 tends to increase when  $\theta_v$  increases. However, in these simulations, this increase is less  
 457 important than for 1D because the viewing direction is parallel to the maize rows and therefore  
 458 the soil, that does not emit SIF, keeps to be seen by the sensor when  $\theta_v$  increases. As with the  
 459 homogeneous canopy, local bioclimatology (*i.e.*,  $\eta$  factors) greatly influences SIF emission,  
 460 and therefore the canopy SIF radiance. Also, at 0.01m resolution, DART-Lux deduces by  $\approx 50$   
 461 the memory usage and simulation time of DART-FT.

462 *Tree plot:* the pixel-wise RMSE (Figure 9) of the DART-Lux and DART-FT SIF radiance  
 463 images decreases with the number of samples/pixel in DART-Lux. This is explained by the  
 464 decrease of the Monte Carlo noise in DART-Lux. For example, the pixel-wise MARD  
 465 decreases from 16.89% for 200 samples/pixel down to 13.88% with 1000 samples/pixel. Here,  
 466 convergence occurs for  $\approx 1000$  samples/pixel. The optimal number of samples/pixel depends  
 467 on several factors including the expected accuracy on scene radiance, and the spatial extent and  
 468 complexity of the studied landscape. The accuracy of the representation of the 3D landscape  
 469 should also be considered.

470 Because Monte Carlo-based radiative transfer models are expected to be more accurate than  
 471 discrete ordinate models, and because the BDPT algorithm is unbiased (Wang et al., 2022), the  
 472 convergence of  $\text{RMSE}_{\text{DART-FT-DART-Lux}}$  is probably an indication of the accuracy of DART-FT,  
 473 with DART-Lux giving the exact value.

474 Results stress that the reduction of simulation time  $\text{CT}_{\text{FT/Lux}} = \frac{\text{DART-FT computer time}}{\text{DART-Lux computer time}}$  of DART-  
 475 Lux relative to DART-FT can be very important, especially for large and complex scenes.  
 476  $\text{CT}_{\text{FT/Lux}} \approx 5800$  for the Ripperdan site. Indeed, the simulation time of DART-FT greatly increases  
 477 with the number of facets, conversely to DART-Lux if the number of samples/pixel remains  
 478 constant. Also,  $\text{CT}_{\text{FT/Lux}}$  decreases with the number of simulated spectral bands. Indeed, the  
 479 DART-FT forward flux tracking simulates SIF with vector-to-matrix products which gives a  
 480 number of multiplication operations proportional to  $N^2$ , with  $N$  the number of spectral bands.  
 481 On the other hand, because DART-Lux path tracing is bi-directional, for rays traced in the  
 482 backward direction, the SIF emission is modelled by a matrix-to-matrix product which gives a  
 483 number of multiplication operations proportional to  $N^3$ . In the absence of SIF simulation,  
 484  $\text{CT}_{\text{FT/Lux}}$  is relatively independent of the number of spectral bands.

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485        Because it usually needs much less RAM than DART-FT for complex scenes especially if it  
486 uses the cloning approach (Wang et al., 2022), DART-Lux is well adapted to large and complex  
487 landscapes for which DART-FT can be inoperative due to hardware constraints. Cloning can  
488 be used for elements of the simulated landscape are identical except for a geometric  
489 transformation: only a single 3D object and a specific geometric transformation (*i.e.*, spatial  
490 shift and scaling-rotation matrix) for each clone are stored in memory. Then, the memory  
491 needed in DART-Lux increases very little with the number of scene elements, conversely to  
492 DART-FT because a geometric transformation matrix usually needs much less memory than a  
493 3D object. Moreover, for DART-Lux, the computation time does not increase a lot when the  
494 scene complexity (*i.e.*, total number of scene facets) increases since the algorithmic complexity  
495 of Monte Carlo methods depend only on the number of samples, conversely to DART-FT where  
496 the total number of tracked rays highly increases with scene complexity. This makes DART-  
497 Lux more computational efficiency for large landscapes, which may be impossible for DART-  
498 FT due to hardware limitations. This is illustrated by the  $3 \times 3 \text{ km}^2$  SIF radiance image of  
499 Ripperdan (Figure 12). Indeed, its simulation only needed 42.9 GB of computer memory and 2  
500 h 44 min of computation time for DART-Lux and was impossible for DART-FT.

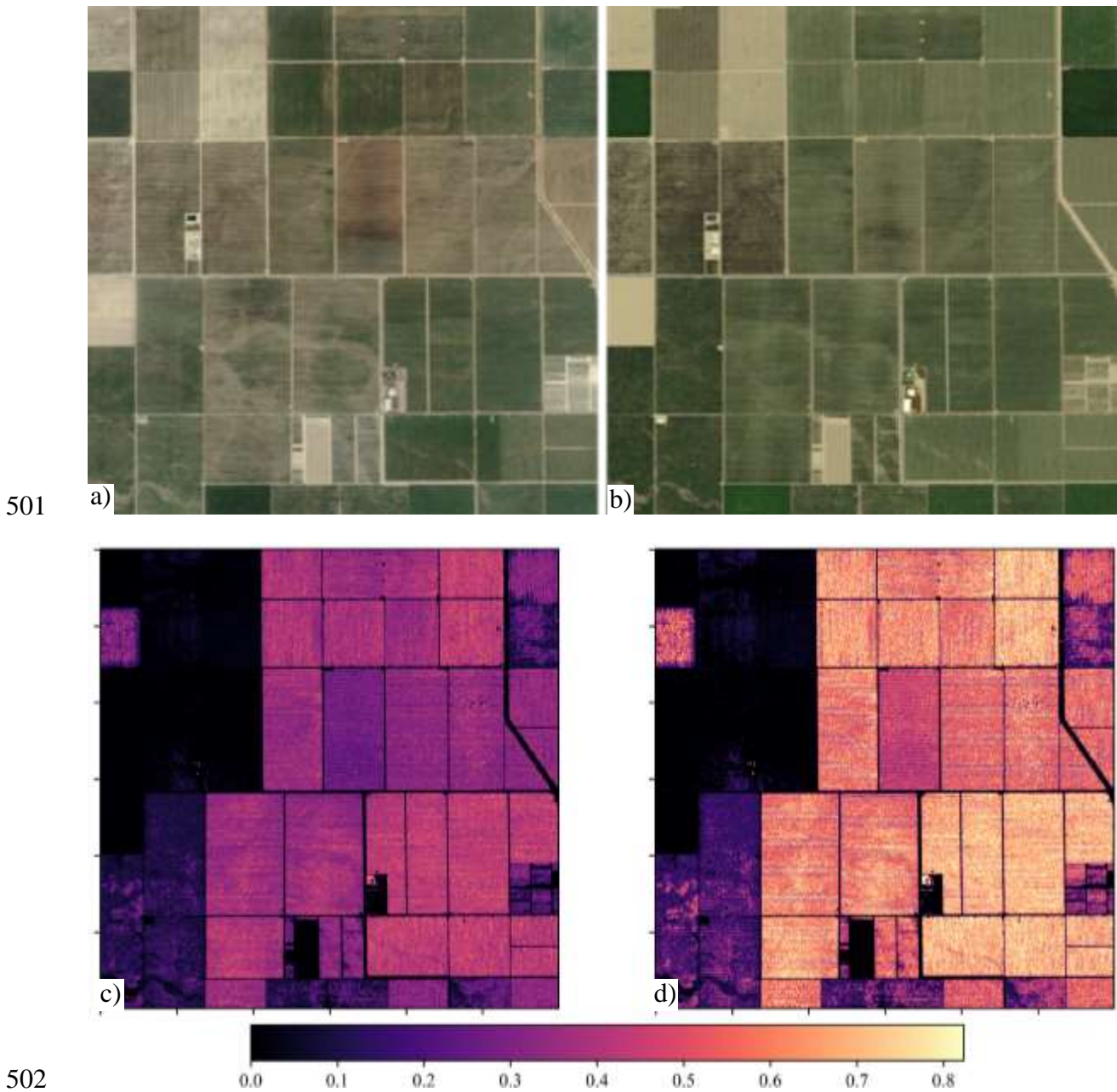


Figure 12. Ripperdan  $3km \times 3km$  agricultural site (vineyards and trees), USA ( $36^{\circ} 55' N$ ,  $119^{\circ} 58' W$ ). a) Google image used to create the DART-Lux's 3D scene. b) DART-Lux RGB color composite. DART-Lux PSI (c) and PSII (d) radiance images ( $W/m^2/\mu m/sr$ ) at  $760 nm$  simulated with 100 bands in  $[0.4\mu m - 0.75\mu m]$ . SIF radiance is null for the road (top right), bare earth fields (top left) and built areas (bottom center). DART-Lux images are at 5m spatial resolution.



511 **VI. Conclusion**

512 We designed a new SIF radiative transfer modelling that adapts the equations governing the  
513 SIF emission to the Bidirectional Path Tracing (BDPT) algorithm (Veach, 1998) that constructs  
514 light paths from the light source and from the sensor. This is a novel SIF modelling approach.  
515 Indeed, apart from DART-Lux, to our knowledge, all Monte Carlo RT models that simulate  
516 SIF (*e.g.*, FLiES-SIF, FluorFLIGHT, FluorWPS, FluCVRT) use forward tracing, although the  
517 BDPT algorithm is more powerful for simulating SIF images. Adapting the BDPT algorithm to  
518 SIF modelling greatly improves the efficiency of DART for SIF images simulation, due to the  
519 efficiency of backward tracing, especially for sensors with narrow fields of view (Disney et al.,  
520 2000).

521 For that, we adapted the equations that allow to compute the SIF emission for the BDPT  
522 algorithms. The new equations allow to compute the radiance starting both from the light source  
523 and from the sensor, and to obtain the total signal (scattered + emitted SIF radiance) in addition  
524 to the SIF radiance components per photosystem separately. Simulations conducted with simple  
525 3D canopies illustrated that DART-Lux and DART-FT SIF images have a good agreement. In  
526 addition, DART-Lux and 1D SCOPE gave similar total and SIF radiance values when using a  
527 very similar scene representation (*i.e.*, homogeneous turbid medium and quasi-turbid medium).  
528 They tend to greatly differ if the 3D architecture of the studied landscape is considered. To  
529 account for the effect of local climatological conditions (*e.g.*, leaf temperature) on leaf-level  
530 SIF emission, DART-Lux can be coupled with the 1D energy balance module of SCOPE by  
531 importing vertical profiles of  $\eta$  factors, similarly to DART-FT (Malenovský et al., 2021).

532 Compared to DART-FT, DART-Lux SIF modelling greatly decreases computational needs  
533 (*i.e.*, RAM and computer time). This decrease was  $\approx 50$  for the maize field with a spatial  
534 resolution equal to 0.01m, and was larger than  $10^3$  for the  $3 \times 3 \text{ km}^2$  Ripperdan agricultural  
535 site zone. This makes DART a powerful model to simulate SIF images of large and complex  
536 landscapes, with many spectral bands. It opens new horizons for RS studies of vegetation. The  
537 novel SIF simulation in DART-Lux is already in the released DART versions (v1152 onwards)  
538 (<https://dart.omp.eu>).

539

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 543 National de la Recherche Scientifique) through the 80|Prime program.

544

545 **Appendix 1. Block matrices product**

546 The product of the block matrices  $M_1 = \begin{pmatrix} A_1 & B_1 & C_1 \\ 0 & D_1 & 0 \\ 0 & 0 & D_1 \end{pmatrix}$  and  $M_2 = \begin{pmatrix} A_2 & B_2 & C_2 \\ 0 & D_2 & 0 \\ 0 & 0 & D_2 \end{pmatrix}$ , with  $D_1$

547 and  $D_2$  diagonal matrices, is a block matrix with same form as  $M_1$  and  $M_2$ :

548 
$$M_1 \times M_2 = \begin{pmatrix} A_1 & B_1 & C_1 \\ 0 & D_1 & 0 \\ 0 & 0 & D_1 \end{pmatrix} \times \begin{pmatrix} A_2 & B_2 & C_2 \\ 0 & D_2 & 0 \\ 0 & 0 & D_2 \end{pmatrix} = \begin{pmatrix} A_1 \cdot A_2 & A_1 B_2 + B_1 D_2 & A_1 C_2 + C_1 D_2 \\ 0 & D_1 D_2 & 0 \\ 0 & 0 & D_1 D_2 \end{pmatrix}$$

549 with  $D_1 D_2$  a diagonal matrix.

550

551 **References**

- 552 Braghieri, R. K., Wang, Y., Doughty, R., Sousa, D., Magney, T., Widlowski, J.-L., Longo,  
553 M., Bloom, A. A., Worden, J., Gentine, P., & Frankenberg, C. (2021). Accounting for  
554 canopy structure improves hyperspectral radiative transfer and sun-induced  
555 chlorophyll fluorescence representations in a new generation Earth System model.  
556 *Remote Sensing of Environment*, 261, 112497.  
557 <https://doi.org/10.1016/j.rse.2021.112497>
- 558 Cormen, T. H., Leiserson, C. E., Rivest, R. L., & Stein, C. (2009). *Introduction to Algorithms*  
559 (3rd ed.). MIT Press.
- 560 Damm, A., Guanter, L., Paul-Limages, E., Tol, C. van der, Hueni, A., Buchmann, N., Eugster,  
561 W., Ammann, C., & Schaepman, M. E. (2015). Far-red sun-induced chlorophyll  
562 fluorescence shows ecosystem - specific relationships to gross primary production: An  
563 assessment based on observational and modeling approaches. *Remote Sensing of*  
564 *Environment*, 166, 91–105. <https://doi.org/10.1016/j.rse.2015.06.004>
- 565 Disney, M. I., Lewis, P., & North, P. R. J. (2000). Monte Carlo ray tracing in optical canopy  
566 reflectance modelling. *Remote Sensing Reviews*, 18(2–4), 163–196.  
567 <https://doi.org/10.1080/02757250009532389>
- 568 Gastellu-Etchegorry, J.-P., Demarez, V., Pinel, V., & Zagolski, F. (1996). Modeling radiative  
569 transfer in heterogeneous 3-D vegetation canopies. *Remote Sensing of Environment*,  
570 58(2), 131–156. [https://doi.org/10.1016/0034-4257\(95\)00253-7](https://doi.org/10.1016/0034-4257(95)00253-7)
- 571 Guanter, L., Zhang, Y., Jung, M., Joiner, J., Voigt, M., Berry, J. A., Frankenberg, C., Huete,  
572 A. R., Zarco-Tejada, P., Lee, J.-E., Moran, M. S., Ponce-Campos, G., Beer, C.,  
573 Camps-Valls, G., Buchmann, N., Gianelle, D., Klumpp, K., Cescatti, A., Baker, J. M.,  
574 & Griffis, T. J. (2014). Global and time-resolved monitoring of crop photosynthesis  
575 with chlorophyll fluorescence. *Proceedings of the National Academy of Sciences*,  
576 111(14), E1327–E1333. <https://doi.org/10.1073/pnas.1320008111>
- 577 Hernández-Clemente, R., North, P. R. J., Hornero, A., & Zarco-Tejada, P. J. (2017).  
578 Assessing the effects of forest health on sun-induced chlorophyll fluorescence using  
579 the FluorFLIGHT 3-D radiative transfer model to account for forest structure. *Remote*  
580 *Sensing of Environment*, 193, 165–179. <https://doi.org/10.1016/j.rse.2017.02.012>

- 581 Hornero, A., North, P. R. J., Zarco-Tejada, P. J., Rascher, U., Martín, M. P., Migliavacca, M.,  
 582 & Hernandez-Clemente, R. (2021). Assessing the contribution of understory sun-  
 583 induced chlorophyll fluorescence through 3-D radiative transfer modelling and field  
 584 data. *Remote Sensing of Environment*, 253, 112195.  
 585 <https://doi.org/10.1016/j.rse.2020.112195>
- 586 Kallel, A. (2020). FluLCVRT: Reflectance and fluorescence of leaf and canopy modeling  
 587 based on Monte Carlo vector radiative transfer simulation. *Journal of Quantitative*  
 588 *Spectroscopy and Radiative Transfer*, 253, 107183.  
 589 <https://doi.org/10.1016/j.jqsrt.2020.107183>
- 590 Kalos, M. H., & Whitlock, P. A. (1986). *Monte Carlo methods. Vol. 1: Basics*. Wiley-  
 591 Interscience.
- 592 Liu, W., Atherton, J., Möttus, M., Gastellu-Etchegorry, J.-P., Malenovský, Z., Raunonen, P.,  
 593 Åkerblom, M., Mäkipää, R., & Porcar-Castell, A. (2019). Simulating solar-induced  
 594 chlorophyll fluorescence in a boreal forest stand reconstructed from terrestrial laser  
 595 scanning measurements. *Remote Sensing of Environment*, 232, 111274.  
 596 <https://doi.org/10.1016/j.rse.2019.111274>
- 597 Liu, W., Luo, S., Lu, X., Atherton, J., & Gastellu-Etchegorry, J.-P. (2020). Simulation-Based  
 598 Evaluation of the Estimation Methods of Far-Red Solar-Induced Chlorophyll  
 599 Fluorescence Escape Probability in Discontinuous Forest Canopies. *Remote Sensing*,  
 600 12(23), Article 23. <https://doi.org/10.3390/rs12233962>
- 601 Liu, X., Guanter, L., Liu, L., Damm, A., Malenovský, Z., Rascher, U., Peng, D., Du, S., &  
 602 Gastellu-Etchegorry, J.-P. (2019). Downscaling of solar-induced chlorophyll  
 603 fluorescence from canopy level to photosystem level using a random forest model.  
 604 *Remote Sensing of Environment*, 231, 110772.  
 605 <https://doi.org/10.1016/j.rse.2018.05.035>
- 606 Malenovský, Z., Regaieg, O., Yin, T., Lauret, N., Guilleux, J., Chavanon, E., Duran, N.,  
 607 Janoutová, R., Delavois, A., Meynier, J., Medjdoub, G., Yang, P., van der Tol, C.,  
 608 Morton, D., Cook, B. D., & Gastellu-Etchegorry, J.-P. (2021). Discrete anisotropic  
 609 radiative transfer modelling of solar-induced chlorophyll fluorescence: Structural  
 610 impacts in geometrically explicit vegetation canopies. *Remote Sensing of*  
 611 *Environment*, 263, 112564. <https://doi.org/10.1016/j.rse.2021.112564>

### 3.1 VEGETATION SIMULATED AS FACETS

- 612 Miller, J. (2005). *Development of a Vegetation Fluorescence Canopy Model*.
- 613 Mohammed, G. H., Colombo, R., Middleton, E. M., Rascher, U., van der Tol, C., Nedbal, L.,  
614 Goulas, Y., Pérez-Priego, O., Damm, A., Meroni, M., Joiner, J., Cogliati, S., Verhoef,  
615 W., Malenovský, Z., Gastellu-Etchegorry, J.-P., Miller, J. R., Guanter, L., Moreno, J.,  
616 Moya, I., ... Zarco-Tejada, P. J. (2019). Remote sensing of solar-induced chlorophyll  
617 fluorescence (SIF) in vegetation: 50 years of progress. *Remote Sensing of*  
618 *Environment*, 231, 111177. <https://doi.org/10.1016/j.rse.2019.04.030>
- 619 Nicodemus, F. E. (Fred E. (1978). *Self-study manual on optical radiation measurements: Part*  
620 *I-Concepts, Chapters 4 and 5*. National Bureau of Standards (U.S.).  
621 <http://archive.org/details/selfstudymanualo9102nico>
- 622 Pharr, M., Jakob, W., & Humphreys, G. (2016). *Physically Based Rendering: From Theory to*  
623 *Implementation* (3rd ed.). Morgan Kaufmann Publishers Inc.
- 624 Porcar-Castell, A., Tyystjärvi, E., Atherton, J., van der Tol, C., Flexas, J., Pfündel, E. E.,  
625 Moreno, J., Frankenberg, C., & Berry, J. A. (2014). Linking chlorophyll a  
626 fluorescence to photosynthesis for remote sensing applications: Mechanisms and  
627 challenges. *Journal of Experimental Botany*, 65(15), 4065–4095.  
628 <https://doi.org/10.1093/jxb/eru191>
- 629 Regaieg, O., Yin, T., Malenovský, Z., Cook, B. D., Morton, D. C., & Gastellu-Etchegorry, J.-  
630 P. (2021). Assessing impacts of canopy 3D structure on chlorophyll fluorescence  
631 radiance and radiative budget of deciduous forest stands using DART. *Remote Sensing*  
632 *of Environment*, 265, 112673. <https://doi.org/10.1016/j.rse.2021.112673>
- 633 Rosema, A., Verhoef, W., Schroote, J., & Snel, J. F. H. (1991). Simulating fluorescence light-  
634 canopy interaction in support of laser-induced fluorescence measurements. *Remote*  
635 *Sensing of Environment*, 37(2), 117–130. [https://doi.org/10.1016/0034-](https://doi.org/10.1016/0034-4257(91)90023-Y)  
636 [4257\(91\)90023-Y](https://doi.org/10.1016/0034-4257(91)90023-Y)
- 637 Sakai, Y., Kobayashi, H., & Kato, T. (2020). FLiES-SIF version 1.0: Three-dimensional  
638 radiative transfer model for estimating solar induced fluorescence. *Geoscientific*  
639 *Model Development*, 13(9), 4041–4066. <https://doi.org/10.5194/gmd-13-4041-2020>
- 640 Song, L., Guanter, L., Guan, K., You, L., Huete, A., Ju, W., & Zhang, Y. (2018). Satellite  
641 sun-induced chlorophyll fluorescence detects early response of winter wheat to heat

- 642 stress in the Indian Indo-Gangetic Plains. *Global Change Biology*, 24(9), 4023–4037.  
 643 <https://doi.org/10.1111/gcb.14302>
- 644 van der Tol, C., Verhoef, W., Timmermans, J., Verhoef, A., & Su, Z. (2009). An integrated  
 645 model of soil-canopy spectral radiances, photosynthesis, fluorescence, temperature  
 646 and energy balance. *Biogeosciences*, 6(12), 3109–3129. [https://doi.org/10.5194/bg-6-](https://doi.org/10.5194/bg-6-3109-2009)  
 647 [3109-2009](https://doi.org/10.5194/bg-6-3109-2009)
- 648 Veach, E. (1998). *Robust monte carlo methods for light transport simulation* [Phd]. Stanford  
 649 University.
- 650 Veach, E., & Guibas, L. J. (1995). Optimally combining sampling techniques for Monte Carlo  
 651 rendering. *Proceedings of the 22nd Annual Conference on Computer Graphics and*  
 652 *Interactive Techniques*, 419–428. <https://doi.org/10.1145/218380.218498>
- 653 Verhoef, W. (1984). Light scattering by leaf layers with application to canopy reflectance  
 654 modeling: The SAIL model. *Remote Sensing of Environment*, 16(2), 125–141.  
 655 [https://doi.org/10.1016/0034-4257\(84\)90057-9](https://doi.org/10.1016/0034-4257(84)90057-9)
- 656 Verrelst, J., Malenovsky, Z., Tol, C. van der, Camps-Valls, G., Gastellu-Etchegorry, J.-P.,  
 657 Lewis, P., North, P., & Moreno, J. (2019). Quantifying Vegetation Biophysical  
 658 Variables from Imaging Spectroscopy Data: A Review on Retrieval Methods. *Surveys*  
 659 *in Geophysics*, 40(3), 589–629. <https://doi.org/10.1007/s10712-018-9478-y>
- 660 Vilfan, N., van der Tol, C., Muller, O., Rascher, U., & Verhoef, W. (2016). Fluspect-B: A  
 661 model for leaf fluorescence, reflectance and transmittance spectra. *Remote Sensing of*  
 662 *Environment*, 186, 596–615. <https://doi.org/10.1016/j.rse.2016.09.017>
- 663 Vilfan, N., Van der Tol, C., Yang, P., Wyber, R., Malenovský, Z., Robinson, S. A., &  
 664 Verhoef, W. (2018). Extending Fluspect to simulate xanthophyll driven leaf  
 665 reflectance dynamics. *Remote Sensing of Environment*, 211, 345–356.  
 666 <https://doi.org/10.1016/j.rse.2018.04.012>
- 667 Wang, Y., Kallel, A., Yang, X., Regaieg, O., Lauret, N., Guilleux, J., Chavanon, E., &  
 668 Gastellu-Etchegorry, J.-P. (2022). DART-Lux: An unbiased and rapid Monte Carlo  
 669 radiative transfer method for simulating remote sensing images. *Remote Sensing of*  
 670 *Environment*, 274, 112973. <https://doi.org/10.1016/j.rse.2022.112973>

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- 671 Wang, Y., Lauret, N., & Gastellu-Etchegorry, J.-P. (2020). DART radiative transfer  
672 modelling for sloping landscapes. *Remote Sensing of Environment*, 247, 111902.  
673 <https://doi.org/10.1016/j.rse.2020.111902>
- 674 Yang, P., Verhoef, W., & van der Tol, C. (2017). The mSCOPE model: A simple adaptation  
675 to the SCOPE model to describe reflectance, fluorescence and photosynthesis of  
676 vertically heterogeneous canopies. *Remote Sensing of Environment*, 201, 1–11.  
677 <https://doi.org/10.1016/j.rse.2017.08.029>
- 678 Zhang, Z., Zhang, Y., Porcar-Castell, A., Joiner, J., Guanter, L., Yang, X., Migliavacca, M.,  
679 Ju, W., Sun, Z., Chen, S., Martini, D., Zhang, Q., Li, Z., Cleverly, J., Wang, H., &  
680 Goulas, Y. (2020). Reduction of structural impacts and distinction of photosynthetic  
681 pathways in a global estimation of GPP from space-borne solar-induced chlorophyll  
682 fluorescence. *Remote Sensing of Environment*, 240, 111722.  
683 <https://doi.org/10.1016/j.rse.2020.111722>
- 684 Zhao, F., Dai, X., Verhoef, W., Guo, Y., van der Tol, C., Li, Y., & Huang, Y. (2016).  
685 FluorWPS: A Monte Carlo ray-tracing model to compute sun-induced chlorophyll  
686 fluorescence of three-dimensional canopy. *Remote Sensing of Environment*, 187, 385–  
687 399. <https://doi.org/10.1016/j.rse.2016.10.036>  
688

## 3.2 Vegetation simulated as turbid medium

The LuxCoreRender software can simulate the propagation of radiation in volumes filled with fluids. It uses the Schlick phase function in order to approximate the Henyey-Greenstein phase function commonly used in DART for simulating scattering by aerosols in the atmosphere. The Schlick phase function is more convenient for computer graphics because it is faster to compute, although it is less accurate. Based on this implementation, I introduced into DART-Lux (1) the double Henyey-Greenstein and the Rayleigh scattering phase functions in order to simulate radiation propagation in fluids, as in DART-FT, then (2) turbid vegetation modeling, including SIF modeling. The modeling approach is presented below, after the introduction of the Light Transport Equation generalized for scenes containing surfaces and scattering media volumes.

### 3.2.1 Modeling approach

#### *Generalized Light Transport Equation*

The surface form of the Light Transport Equation gives the radiance reaching a vertex  $p$  from a surface  $A$ , after being scattered at a vertex  $p'$  on a surface  $\Sigma$  (here, emission is omitted):

$$L(p' \rightarrow p) = \int_A f(p'' \rightarrow p' \rightarrow p) \cdot L(p'' \rightarrow p') \cdot G(p'' \leftrightarrow p') \cdot dA(p'') \quad (3.1)$$

$$\text{with } G(p'' \leftrightarrow p') = V(p'' \leftrightarrow p') \cdot \frac{|\cos\theta_0''| \cdot |\cos\theta_i'|}{\|p' - p''\|^2},$$

$f(p'' \rightarrow p' \rightarrow p)$ : BSDF of surface  $\Sigma$ ,

$L(p'' \rightarrow p')$ : radiance reaching  $p'$  from  $p''$ ,

$V$ : binary visibility function,

$$\cos\theta_0'' = \vec{n}'' \cdot \frac{\overrightarrow{p''p'}}{\|p' - p''\|}, \quad \cos\theta_i' = \frac{\overrightarrow{p''p'}}{\|p' - p''\|} \cdot \vec{n}',$$

$\vec{n}'$  and  $\vec{n}''$ : normal vectors to the surface  $\Sigma$  at  $p'$  and to the surface  $A$  at  $p''$  respectively.

To allow the simulation of volumes, the Light Transport Equation is generalized for scenes including scattering surfaces and volume scattering media:

### 3.2 VEGETATION SIMULATED AS TURBID MEDIUM

$$L(p' \rightarrow p) = \int_A \hat{f}(p'' \rightarrow p' \rightarrow p) \cdot L(p'' \rightarrow p') \cdot \hat{G}(p'' \leftrightarrow p') \cdot dA(p'') \quad (3.2)$$

$$\text{with } \hat{f}(p'' \rightarrow p' \rightarrow p) = \begin{cases} \frac{\sigma_s}{\sigma_s + \sigma_a} \cdot p_s(p'' \rightarrow p' \rightarrow p), & \text{if } p' \text{ is a volume vertex} \\ f(p'' \rightarrow p' \rightarrow p), & \text{if } p' \text{ is a surface vertex} \end{cases}$$

$\sigma_s$ , and  $\sigma_a$ : scattering and absorption extinction coefficients of the volume,

$p_s(p'' \rightarrow p' \rightarrow p)$ : normalized scattering phase function of the volume,

$$\hat{G}(p'' \leftrightarrow p') = V(p'' \leftrightarrow p') \cdot Tr(p' \rightarrow p'') \cdot \frac{C(p', p'') \cdot C(p'', p')}{\|p' - p''\|^2},$$

$Tr(p' \rightarrow p'')$ : path transmittance between  $p'$  and  $p''$ ,

$$C(p, p') = \begin{cases} \left| \vec{n}_p \cdot \frac{\overline{pp'}}{\|p - p'\|} \right|, & \text{if } p \text{ is a surface vertex} \\ 1, & \text{if } p \text{ is a volume vertex} \end{cases}.$$

#### **Monte-Carlo path tracing (Fluids analogy)**

In radiative transfer theory, fluids are usually assumed to have a sufficiently high particle density to be treated statistically using the Beer law. Also, the density of particles is assumed not to be too large in order to ensure that the absorbance of the fluid is proportional to the fluid density. Because the turbid medium model is similar to the fluid model, and because the fluids are simpler to treat using their analytical phase functions in the frame of Monte-Carlo path tracing, fluids modeling is presented first, then, turbid modeling is derived from it.

Monte-Carlo path tracing aims to randomly sample light paths by ensuring that the most probable paths have higher chances to be sampled. For fluid volumes, this is done in two steps:

##### *a) Sampling a traveling distance*

A ray entering a fluid volume is partly transmitted. The Beer law gives the direct transmittance:

$$T_t(\Delta L) = e^{-\sigma_t \Delta L} \quad (3.3)$$

with  $\Delta L$  the travel distance and  $\sigma_t = \sigma_s + \sigma_a$  the total extinction coefficient ( $\text{m}^2$  of interceptor /  $\text{m}^3$ ).  $\sigma_t$  is the sum of scattering and absorption extinction coefficients.

Here, it is assumed to be isotropic.

Complementarily, the probability that a ray is intercepted after a travel distance less or equal than  $\Delta L$  is  $1 - T_t(\Delta L)$ . It is the Cumulative Distribution Function (CDF)  $P_{\sigma_t}(\Delta L)$  that an



interception occurs at a distance  $l \leq \Delta L$ , which is the integral of the Probability Density Function (PDF)  $p_{\sigma_t}(l)$  that an interception occurs at a distance  $l$  per distance unit:

$$P_{\sigma_t}(\Delta L) = \int_0^{\Delta L} p_{\sigma_t}(l) \cdot dl = 1 - e^{-\sigma_t \Delta L} \quad (3.4)$$

$$p_{\sigma_t}(l) = \frac{dP_{\sigma_t}(l)}{dl} = \sigma_t \cdot e^{-\sigma_t l} \quad (3.5)$$

Sampling  $p_{\sigma_t}(l)$  gives a sampled travel distance  $\Delta l$  in the medium. The inversion method (cf. Appendix 3-1) is used to draw a random sample  $u$  from a given PDF  $p(x)$ : the inverse function of its CDF is applied to a random number  $\xi$  uniformly sampled between 0 and 1. Hence, the travel distance  $\Delta l$  through the medium is sampled using a random number  $\xi \sim \mathcal{U}([0,1])$ :

$$\Delta l = P_{\sigma_t}^{-1}(\xi) = -\frac{\ln(1 - \xi)}{\sigma_t} \quad (3.6)$$

If  $\Delta l < \Delta L$ , with  $\Delta L$  the pathlength needed by the ray to exit the medium, the ray is scattered after the pathlength  $\Delta l$ . If  $\Delta l > \Delta L$ , the ray is transmitted through the medium.

In fluids, the extinction coefficients usually vary with the wavelength. For a multiband ray,  $\Delta l$  is sampled using the spectral average  $\bar{\sigma}_t$  over all bands. Then, if a ray is intercepted (i.e.,  $\Delta l < \Delta L$ ), its transmittance  $Tr_{ray,int}$  is null for all spectral bands, and if a ray is transmitted ( $\Delta l \geq \Delta L$ ), its transmittance  $Tr_{ray,trans}$  is 1 for all spectral bands. The expected value of the transmittance for all spectral bands can be written:

$$E[Tr(\bar{\sigma}_t, \Delta L)] = \int_0^{\Delta L} 0 \cdot p_{\bar{\sigma}_t}(l) dl + \int_{\Delta L}^{+\infty} 1 \cdot p_{\bar{\sigma}_t}(l) dl = e^{-\bar{\sigma}_t \Delta L} \quad (3.7)$$

The obtained expected transmittance is a transmittance corresponding to the averaged  $\bar{\sigma}_t$  for all spectral bands. A transmittance correction factor  $f = \frac{e^{-\sigma_t \Delta L}}{e^{-\bar{\sigma}_t \Delta L}}$  is applied per spectral band in order to get the correct expected transmittance for each spectral band:

$$E[Tr(\bar{\sigma}_t, \sigma_t, \Delta L)] = \int_{\Delta L}^{+\infty} \frac{e^{-\sigma_t \Delta L}}{e^{-\bar{\sigma}_t \Delta L}} \cdot p_{\bar{\sigma}_t}(l) dl = \frac{e^{-\sigma_t \Delta L}}{e^{-\bar{\sigma}_t \Delta L}} \cdot e^{-\bar{\sigma}_t \Delta L} = e^{-\sigma_t \Delta L} \quad (3.8)$$

If an interception occurs, the intercepted ray is scattered with a radiance multiplied by the albedo  $\frac{\sigma_s}{\sigma_t}$  because part of the intercepted ray is absorbed.

### 3.2 VEGETATION SIMULATED AS TURBID MEDIUM

For turbid medium, the extinction coefficient  $\sigma_t(\Omega_s)$  depends on the incident direction. It is isotropic only if the Leaf Angular Distribution is spherical:

$$\sigma_t(\Omega_s) = G(\Omega_s) \cdot u_l \quad (3.9)$$

$$\text{with } G(\Omega_s) = \int_0^{\frac{\pi}{2}} \frac{g(\theta_l)}{2\pi} \int_0^{2\pi} |\Omega_l \cdot \Omega_s| \cdot d\phi_l \cdot \sin\theta_l \cdot d\theta_l,$$

$u_l$  the leaf volume density and

$\frac{g(\theta_l)}{2\pi}$  the Leaf Angular Distribution function.

The PDF of interception and scattering of a ray after a travel path  $l$  through the medium is:

$$p(l, \Omega_s) = G(\Omega_s) \cdot u_l \cdot e^{-G(\Omega_s) \cdot u_l \cdot l} \quad (3.10)$$

The extinction coefficient  $\sigma_t = G(\Omega_s) \cdot u_l$  does not depend on wavelength. Hence, the transmittance correction factor  $f$  applied for fluids is not needed.

Being a function of the direction  $\Omega_s$ , the term  $G$  must be computed per traced direction. Because its computation on the fly is computationally expensive,  $G$  is precomputed for  $N$  discrete directions. Then, since any direction can be sampled,  $G$  is interpolated using the values for the directions that neighbor the sampled direction. If a volume contains several types of turbid/fluid medium, the sampling of distance is done using an equivalent extinction coefficient that is the sum of the extinction coefficients of all the elements in the volume.

Radiation reflected by vegetation covers has usually a sharp maximum in the retro-illumination direction. Indeed, shadows cast by the leaves in the incident direction cannot be seen in this direction because they are hidden by the leaves themselves. For directions close to the retro-illumination direction, shadows can be observed, which usually translates in a decrease of reflectance. This is known as the hot spot effect. The approach of Kuusk, (1985) is widely used to model the hot spot effect. In the standard DART model (*i.e.*, DART-FT), Gastellu-Etchegorry et al. (1996) adapted the approach of Kuusk (1985) to finite dimensions turbid cells. Although some hot spot models are more accurate (Gobron et al., 1997; Kallel & Nilson, 2013), the Kuusk model is selected for DART-Lux because of its simplicity and adaptability to the Monte Carlo method. For example, Antyufeev & Marshak (1990) used it in their Monte Carlo model. DART-FT also uses it, which eases comparison with DART-Lux.

For a viewing direction  $\Omega_v$  such that  $\Omega_s \cdot \Omega_v < 0$  and a path length  $\Delta l$ , the transmittance is no longer  $Tr(\Delta l, \Omega_v) = e^{-u_l \cdot G(\Omega_v) \cdot \Delta l}$ . It is (cf. Appendix 3-2):

$$Tr(\Delta l, \Omega_s \rightarrow \Omega_v) = e^{-u_l \cdot G(\Omega_v) \cdot (\Delta l + \frac{\beta}{\alpha}(e^{-\alpha \Delta l} - 1))} = e^{-\zeta \cdot \phi(\Delta l)} \quad (3.11)$$

$$\text{with: } \alpha = \frac{\Delta(\Omega_s, \Omega_v) \cdot |\mu_v|}{S_l}, \beta = \sqrt{\frac{G(\Omega_s) \cdot |\mu_v|}{G(\Omega_v) \cdot |\mu_s|}}, \Delta(\Omega_s, \Omega_v) = \sqrt{\frac{1}{\mu_v^2} + \frac{1}{\mu_s^2} + \frac{2 \cdot \Omega_s \cdot \Omega_v}{|\mu_s \cdot \mu_v|}}, \mu_s = \cos \theta_s, \mu_v = \cos \theta_v,$$

$$S_l = \frac{\pi \cdot d_l \cdot G(\Omega_v)}{4 \cdot \mu_v \cdot \int_{2\pi} \int_{\frac{\pi}{2}} \frac{g(\Omega_l)}{2\pi} \cdot \frac{\sin \theta_l \cdot d\theta_l \cdot d\phi_l}{\sqrt{1 + \tan^2 \theta_l \cdot \sin^2 \theta_l}}}, d_l \text{ the leaf dimension, } u_l \text{ the leaf volume density.}$$

$$\zeta = u \cdot G(\Omega_v), \text{ and } \phi(\Delta l) = \Delta l + \frac{\beta}{\alpha}(e^{-\alpha \Delta l} - 1), \text{ which is positive because } Tr(\Delta l, \Omega_s \rightarrow \Omega_v) \leq 1.$$

With the notation  $x = \phi(\Delta l)$ , the transmittance is written:

$$Tr(x, \Omega_s \rightarrow \Omega_v) = e^{-\zeta \cdot x} \quad (3.12)$$

The PDF of the random variable  $X$  for sampling  $x$  in  $Tr(x, \Omega_s \rightarrow \Omega_v)$  is:

$$p_X(x) = \zeta \cdot e^{-\zeta \cdot x} \quad (3.13)$$

The CDF of the random variable  $X$  is:

$$P_X(x) = 1 - e^{-\zeta \cdot x} \quad (3.14)$$

The CDF of the random variable  $L$ , for sampling a travel distance  $l$  in the hot spot configuration, knowing that the function  $\phi$  is strictly increasing in the range of interest (cf. Appendix 3-3), is:

$$P_L(l) = p(L \leq l) = P(X \leq \phi(l)) = P_X(\phi(l)) = \zeta \cdot e^{-\zeta \cdot \phi(l)} \quad (3.15)$$

The PDF of the random variable  $L$  is then:

$$p_L(l) = \frac{dP_L(l)}{dl} = -\frac{d\phi(l)}{dl} \cdot \zeta^2 \cdot e^{-\zeta \cdot \phi(l)} \quad (3.16)$$

To sample  $l$ , with  $\xi \sim \mathcal{U}([0,1])$

$$x = \phi(l) = -\frac{\ln(1 - \xi)}{\zeta} \leftrightarrow l = \phi^{-1}\left(-\frac{\ln(1 - \xi)}{\zeta}\right) \quad (3.17)$$

The expression of  $\phi^{-1}$  is computed in Appendix 3-3.

### b) Sampling a scattering direction

The scattering direction is sampled according to the scattering phase function  $p(\mu)$ , which is the angular distribution of scattered radiation, with  $\mu = \cos \theta$  and  $\theta$  the angle between the incident and outgoing directions. The sampled direction is defined by 2 angles: the angle  $\theta$  between the incident and outgoing rays, and an azimuthal angle  $\varphi$  in the plane perpendicular to

### 3.2 VEGETATION SIMULATED AS TURBID MEDIUM

the scattered direction. If the scattering phase function is azimuthally symmetric (*i.e.*, depends only on  $\theta$ ), the scattering direction is sampled as:

$$\begin{cases} \cos \theta = P^{-1}(\xi_1) \\ \varphi = 2 \cdot \pi \cdot \xi_2 \end{cases} \quad (3.18)$$

with  $P(x) = \int_{-1}^x p(\mu) d\mu$  the CDF,  $\xi_1 \sim \mathcal{U}([0,1])$  and  $\xi_2 \sim \mathcal{U}([0,1])$ .

#### - Henyey-Greenstein phase function

$$\frac{p(\theta)}{2\pi} = \frac{1}{4\pi} \cdot \frac{1 - g^2}{[1 + g^2 - 2 \cdot g \cdot \cos(\theta)]^{\frac{3}{2}}} \quad (3.19)$$

This phase function is normalized:

$$\int_0^{2\pi} \int_0^\pi \frac{p(\theta)}{2\pi} \cdot \sin(\theta) d\theta d\varphi = 1 \quad (3.20)$$

with the asymmetry parameter  $g \in ]-1,1[$ . It is negative for backward scattering, positive for forward scattering, and null for isotropic scattering.

It can be written as a function of  $\mu = \cos(\theta)$ :

$$p(\mu) = \frac{1}{2} \cdot \frac{1 - g^2}{[1 + g^2 - 2 \cdot g \cdot \mu]^{\frac{3}{2}}} \quad (3.21)$$

Then, we have:

$$\int_{-1}^1 p(\mu) d\mu = 1 \quad (3.22)$$

To sample  $\mu = \cos(\theta)$  from  $p(\mu)$ , we compute the cumulated density function:

$$P(x) = \int_{-1}^x p(\mu) d\mu = \begin{cases} \frac{1 - g^2}{2g} \left[ (1 + g^2 - 2gx)^{-\frac{1}{2}} - \frac{1}{1 + g} \right], & \text{if } g \neq 0 \\ \frac{x + 1}{2}, & \text{if } g = 0 \end{cases} \quad (3.23)$$

The value of  $\mu$  that is sampled is:

$$\mu = \begin{cases} P^{-1}(\xi), & \xi \sim \mathcal{U}([0,1]) \\ \frac{1}{2g} \cdot \left[ 1 + g^2 - \left( \frac{1 - g^2}{1 - g + 2 \cdot g \cdot \xi} \right)^2 \right], & \text{if } g \neq 0 \\ 2 \cdot \xi - 1, & \text{if } g = 0 \end{cases} \quad (3.24)$$

### - Double Henyey-Greenstein phase function

It is a weighted sum of two Henyey-Greenstein phase functions.

$$\frac{p(\theta)}{2\pi} = a \cdot \frac{1}{4\pi} \cdot \frac{1 - g_1^2}{[1 + g_1^2 - 2 \cdot g_1 \cdot \cos(\theta)]^{\frac{3}{2}}} + (1 - a) \cdot \frac{1}{4\pi} \cdot \frac{1 - g_2^2}{[1 + g_2^2 - 2 \cdot g_2 \cdot \cos(\theta)]^{\frac{3}{2}}} \quad (3.25)$$

with  $a \in [0,1]$ . Usually, forward scattering is larger than backward scattering, which corresponds to  $a > 0.5$ . It can be sampled using random numbers  $\xi_1 \sim \mathcal{U}([0,1])$  and  $\xi_2 \sim \mathcal{U}([0,1])$ :

If  $\xi_1 < a$ ,

$$\mu = \begin{cases} \frac{1}{2g_1} \cdot \left[ 1 + g_1^2 - \left( \frac{1 - g_1^2}{1 - g_1 + 2 \cdot g_1 \cdot \xi_2} \right)^2 \right], & \text{if } g_1 \neq 0 \\ 2 \cdot \xi_2 - 1, & \text{if } g_1 = 0 \end{cases} \quad (3.26)$$

Else

$$\mu = \begin{cases} \frac{1}{2g_2} \cdot \left[ 1 + g_2^2 - \left( \frac{1 - g_2^2}{1 - g_2 + 2 \cdot g_2 \cdot \xi_2} \right)^2 \right], & \text{if } g_2 \neq 0 \\ 2 \cdot \xi_2 - 1, & \text{if } g_2 = 0 \end{cases} \quad (3.27)$$

Figure 3-1 shows a test of this sampling method for the case  $a = 0.75$ ,  $g_1 = 0.3$ ,  $g_2 = -0.3$ .

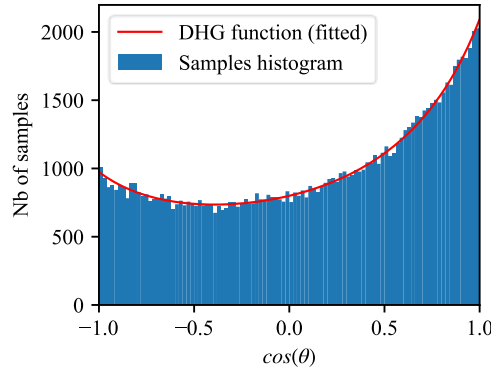


Figure 3-1: Double Henyey-Greenstein phase function sampling test: histogram of  $10^5$  samples and its fitted function ( $a = 0.75$ ,  $g_1 = 0.3$ ,  $g_2 = -0.3$ )

### - Rayleigh phase function

The general form of the Rayleigh scattering phase function is:

$$\frac{p(\theta)}{2\pi} = \frac{1}{4\pi} \cdot [A \cdot (1 + \cos^2(\theta)) + C] \quad (3.28)$$

### 3.2 VEGETATION SIMULATED AS TURBID MEDIUM

The sampling method for the Rayleigh phase function is (cf. Appendix 3-4):

$$\mu = \left( \beta + \sqrt{\alpha^3 + \beta^2} \right)^{\frac{1}{3}} - \frac{\alpha}{\left( \beta + \sqrt{\alpha^3 + \beta^2} \right)^{\frac{1}{3}}} \quad (3.29)$$

with  $\alpha = 1 + \frac{C}{A}$ ,  $\beta = \left( \frac{3}{A} \cdot \xi - \frac{3C}{2A} - 2 \right)$ ,  $\xi \sim \mathcal{U}([0,1])$

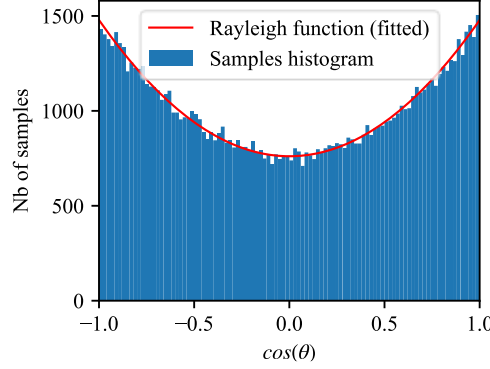


Figure 3-2: Rayleigh phase function sampling test: histogram of  $10^5$  samples and its fitted function ( $A = 0.7175$ ,  $C = 0.0435$ )

The Henyey-Greenstein and Rayleigh scattering phase functions depend only on the cosine of the angle  $\theta$  between the incident and the outgoing directions. Therefore, the incident and outgoing directions play symmetric roles. It explains that these phase functions are adapted to bi-directional modeling with the same PDF used to sample scattering directions for the light and sensor sub-paths.

#### - Turbid vegetation phase function

For a vegetation turbid medium, the scattering transfer function is:

$$T_{scat}(\Omega_s \rightarrow (\Omega_v, \Delta\Omega_v)) = \frac{1}{G(\Omega_s)} \cdot \int_{\Delta\Omega_v} \int_{2\pi} |\Omega_s \cdot \Omega_l| \cdot \frac{g(\Omega_l)}{2\pi} \cdot f(\Omega_l, \Omega_s \rightarrow \Omega_v) \cdot d\Omega_l \cdot d\Omega_v \quad (3.30)$$

where  $f(\Omega_l, \Omega_s \rightarrow \Omega_v)$ : leaf scattering phase function.

$T_{scat}(\Omega_s \rightarrow (\Omega_v, \Delta\Omega_v))$  scattered power  $W_{scat}(\Omega_s \rightarrow \Omega_v)$  in direction  $(\Omega_v, \Delta\Omega_v)$ , per power  $W_{int}(\Delta l_i, \Omega_s)$  intercepted in pathlength  $\Delta l_i$  in direction  $\Omega_s$ .

To define a probability density function (PDF) equivalent to the scattering phase functions for fluids, the PDF of a given direction is assumed to be proportional to the power scattered in this direction. Then, we have:

$$p(\Omega_v|\Omega_s) = \frac{\frac{1}{G(\Omega_s)} \cdot \int_{2\pi} |\Omega_s \cdot \Omega_l| \cdot \frac{g(\Omega_l)}{2\pi} \cdot f(\Omega_f, \Omega_s \rightarrow \Omega_v) \cdot d\Omega_l}{\int_{4\pi} \frac{1}{G(\Omega_s)} \cdot \int_{2\pi} |\Omega_s \cdot \Omega_l| \cdot \frac{g(\Omega_l)}{2\pi} \cdot f(\Omega_l, \Omega_s \rightarrow \Omega_v) \cdot d\Omega_l \cdot d\Omega_v} \quad (3.31)$$

$p(\Omega_v|\Omega_s)$  is normalized:  $\int_{4\pi} p(\Omega_v|\Omega_s) \cdot d\Omega_v = 1$ .

Assuming that the leaves are bi-Lambertian surfaces:

$$p(\Omega_v|\Omega_s) = \frac{\frac{1}{G(\Omega_s)} \cdot \int_{2\pi} |\Omega_s \cdot \Omega_l| \cdot \frac{g(\Omega_l)}{2\pi} \cdot \alpha(\Omega_l, \Omega_s \rightarrow \Omega_v) \cdot |\Omega_v \cdot \Omega_l| d\Omega_l}{\int_{4\pi} \frac{1}{G(\Omega_s)} \cdot \int_{2\pi} |\Omega_s \cdot \Omega_l| \cdot \frac{g(\Omega_l)}{2\pi} \cdot \alpha(\Omega_l, \Omega_s \rightarrow \Omega_v) \cdot |\Omega_v \cdot \Omega_l| d\Omega_l \cdot d\Omega_v} \quad (3.32)$$

$$\text{where: } \alpha(\Omega_l, \Omega_s \rightarrow \Omega_v) = \begin{cases} \frac{\rho_{top}}{\pi} & \text{if } \Omega_l \cdot \Omega_s < 0 \text{ and } \Omega_l \cdot \Omega_v > 0 \\ \frac{\tau_{top}}{\pi} & \text{if } \Omega_l \cdot \Omega_s < 0 \text{ and } \Omega_l \cdot \Omega_v < 0 \\ \frac{\rho_{bot}}{\pi} & \text{if } \Omega_l \cdot \Omega_s > 0 \text{ and } \Omega_l \cdot \Omega_v < 0 \\ \frac{\tau_{bot}}{\pi} & \text{if } \Omega_l \cdot \Omega_s > 0 \text{ and } \Omega_l \cdot \Omega_v > 0 \end{cases}$$

When sampling a scattering direction for a bi-Lambertian surface, the incident and outgoing directions play symmetric roles. For a turbid medium made only of bi-Lambertian surfaces, this symmetry is conserved. Hence, this PDF can be used to sample scattering directions in both direct and reverse directions (*i.e.*, for both light and source sub-paths).

The denominator of Eq (3.32) can be simplified:

$$\begin{aligned} D &= \int_{4\pi} \frac{1}{G(\Omega_s)} \cdot \int_{2\pi} |\Omega_s \cdot \Omega_l| \cdot \frac{g(\Omega_l)}{2\pi} \cdot f(\Omega_l, \Omega_s \rightarrow \Omega_v) \cdot d\Omega_l \cdot d\Omega_v \\ &= \frac{1}{G(\Omega_s)} \cdot \int_{4\pi} f(\Omega_l, \Omega_s \rightarrow \Omega_v) \cdot d\Omega_v \cdot \int_{2\pi} |\Omega_s \cdot \Omega_l| \cdot \frac{g(\Omega_l)}{2\pi} \cdot d\Omega_l \end{aligned} \quad (3.33)$$

The leaf scattering phase function  $f(\Omega_l, \Omega_s \rightarrow \Omega_v)$  verifies:

$$\int_{4\pi} f(\Omega_l, \Omega_s \rightarrow \Omega_v) \cdot d\Omega_v = \omega \quad (3.34)$$

with  $\omega$  is the leaf single scattering albedo.

$\omega = \rho + \tau$ , if the optical properties of the two faces are identical,

$\omega = \frac{1}{2}(\rho_{top} + \rho_{bot}) + \frac{1}{2}(\tau_{top} + \tau_{bot})$ , if the optical properties of the two faces of the leaf differ.

### 3.2 VEGETATION SIMULATED AS TURBID MEDIUM

Then:  $D = \frac{\omega \cdot G(\Omega_s)}{G(\Omega_s)} = \omega$

Finally,

$$p(\Omega_v | \Omega_s) = \frac{1}{\omega \cdot G(\Omega_s)} \cdot \int_{2\pi} |\Omega_s \cdot \Omega_l| \cdot \frac{g(\Omega_l)}{2\pi} \cdot f(\Omega_l, \Omega_s \rightarrow \Omega_v) \cdot d\Omega_l \quad (3.35)$$

Computing this PDF is very expensive. It cannot be solved and sampled analytically using the inversion method directly. Antyufeev & Marshak 1990 used an indirect approach by sampling first a random leaf orientation from the LAD function  $\frac{g(\Omega_f)}{2\pi}$ , then sampling a scattering direction according the leaf BSDF  $f(\Omega_f, \Omega_s \rightarrow \Omega_v)$ . This approach uses a sampling method per LAD function, and implies treating the turbid medium as individual leaves, and not as a whole which increases variance (cf. Section 4.1). Thus, another approach was designed by precomputing the discrete probability distribution for  $N$  discrete direction  $(\Omega_n, \Delta\Omega_n), n \in \{1, \dots, N\}$ :

$$p((\Omega_n, \Delta\Omega_n) | \Omega_s) = \int_{\Delta\Omega_n} p(\Omega_v | \Omega_s) \cdot d\Omega_v \quad (3.36)$$

With the assumption that  $\Delta\Omega_n$  is small enough to consider that the PDF is constant over  $\Delta\Omega_n$ :

$$p((\Omega_n, \Delta\Omega_n) | \Omega_s) = \frac{\Delta\Omega_n}{\omega \cdot G(\Omega_s)} \cdot \int_{2\pi} |\Omega_s \cdot \Omega_l| \cdot \frac{g(\Omega_l)}{2\pi} \cdot f(\Omega_l, \Omega_s \rightarrow \Omega_v) \cdot d\Omega_l \quad (3.37)$$

In DART-FT, the Phase module precomputes the transfer function for the discrete directions:

$$\bar{T}(\lambda, \Omega_s, \Omega_v, \Delta\Omega_v) = \frac{\Delta\Omega_v}{G(\Omega_s)} \cdot \int_{2\pi} |\Omega_s \cdot \Omega_l| \cdot \frac{g(\Omega_l)}{2\pi} \cdot f(\Omega_l, \Omega_s \rightarrow \Omega_v) \cdot d\Omega_l \quad (3.38)$$

This precomputation is used to compute the discrete probability distribution for all outgoing directions, for each incident direction:

$$p((\Omega_n, \Delta\Omega_n) | \Omega_s) = \frac{\bar{T}(\lambda, \Omega_s, \Omega_n, \Delta\Omega_n)}{\omega} \quad (3.39)$$

Then, the PDF for the direction  $\Omega_n$  is given by:

$$p(\Omega_n | \Omega_s) = \frac{\bar{T}(\lambda, \Omega_s, \Omega_n, \Delta\Omega_n)}{\omega \cdot \Delta\Omega_n} \quad (3.40)$$

$p(\Omega_n | \Omega_s)$  is computed for  $N$  ingoing and  $N$  outgoing discrete directions. However, in DART-Lux, rays can propagate in any direction. Therefore, the PDF for any direction is computed with a two-step interpolation. 1) For each neighbor direction of the incident direction, the PDF is



interpolated using the values in neighboring directions of the outgoing direction. 2) Then, results of the first interpolation are interpolated for neighbor directions of the incident direction.

If the volume contains several types of turbid/fluid medium, the scattering direction is determined in two steps. 1) A scattering medium is randomly selected: the probability of selecting a medium is proportional to its scattering extinction coefficient for fluids, and to its extinction coefficient in the incident direction for the turbid medium. 2) Then, a scattering direction is sampled according to the scattering phase function of the selected medium.

### *SIF modeling*

Once the turbid medium is introduced in DART-Lux, modeling the SIF emission in this medium is straightforward using the Monte Carlo path sampling method presented above. Similarly to the scattering phase functions, SIF transfer functions precomputed by the phase module of DART-FT for discrete directions (c.f. Eq (2.5)) are used to evaluate the SIF radiance for the sampled light paths along with the block matrix representation introduced in Section 3.1.

## **3.2.2 Results**

### *Fluids*

The accuracy of fluid modeling in DART-Lux is assessed by comparing DART-Lux and DART-FT nadir images of a parallelepiped fluid volume ( $0.8 \times 0.8 \times 1 \text{ m}^3$ ) over a lambertian surface ( $1 \times 1 \text{ m}^2$ ) of reflectance “loam\_gravelly\_brown\_dark”. Figure 3-3 shows RGB color composites at 2 cm resolution, for two fluid phase functions: a) Double Henyey-Greenstein ( $a = 0.75$ ,  $g_1 = 0.3$ ,  $g_2 = -0.3$ ,  $\sigma_a = 0.4 \text{ m}^2 \cdot \text{m}^{-3}$ ,  $\sigma_s = 0.1 \text{ m}^2 \cdot \text{m}^{-3}$ ), and b) Rayleigh (optical property: “rayleigh\_air”, particle density:  $5 \cdot 10^{29} \text{ m}^{-3}$ ). DART-FT and DART-Lux images are similar with close average reflectance values in the blue, green and red spectral bands (relative differences  $< 1\%$ ). DART-Lux images have some Monte Carlo noise.

### 3.2 VEGETATION SIMULATED AS TURBID MEDIUM

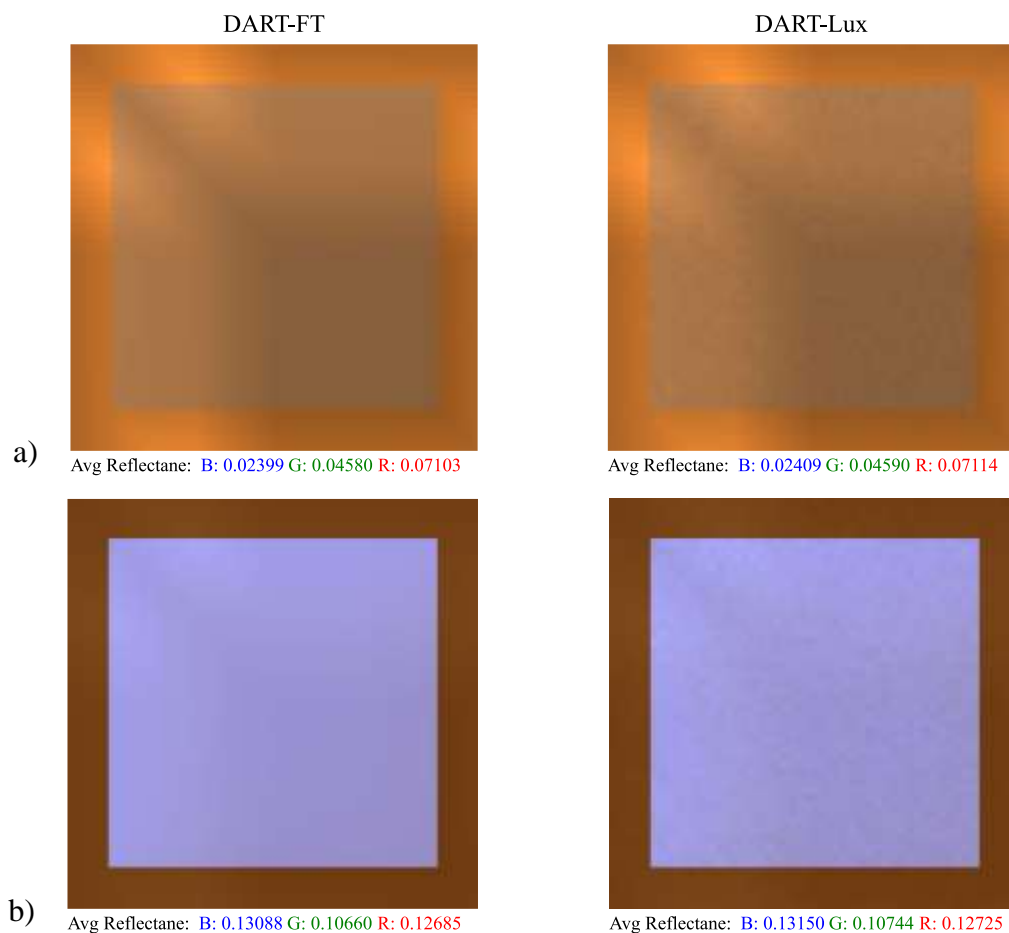


Figure 3-3: DART-FT and DART-Lux RGB nadir images of a fluid volume with fluid phase function double Henyey-Greenstein (a) and Rayleigh (b).

#### ***Turbid medium***

The accuracy of DART-Lux SIF modeling in a turbid medium is assessed by comparison with DART-FT for the case of a turbid volume ( $LAI = 1$ , spherical LAD) over a non-reflective ground and an incident sun radiation with a zenith angle equal to  $30^\circ$ . Figure 3-4 shows the scene total nadir reflectance and scene SIF PSI and PSII nadir radiance simulated by DART-FT and DART-Lux. Figure 3-5 shows the DART-FT and DART-Lux directional reflectance in the solar plane for a near infrared spectral band. The hot spot appears clearly. In both cases, DART-Lux closely agrees with DART-FT: relative difference is 1.21% for reflectance, 0.60% for PSI radiance, and 63% for PSII radiance.

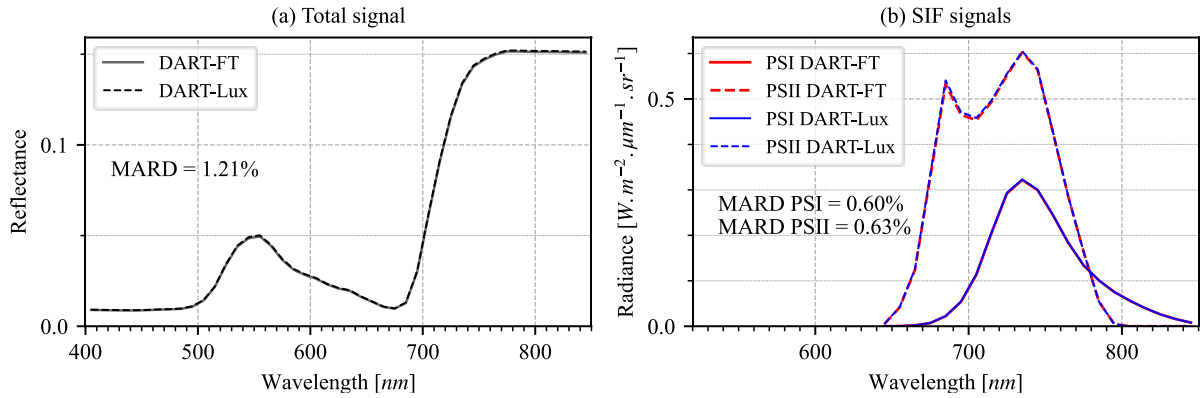


Figure 3-4: Nadir total reflectance and SIF PSI and PSII radiance comparison between DART-FT and DART-Lux for a simple turbid plot

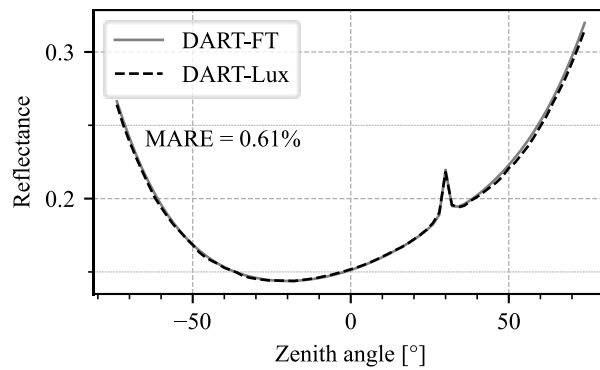


Figure 3-5: Comparison of the directional reflectance for a NIR band in the solar plane between DART-FT and DART-Lux for simple turbid plot

Figure 3-6 shows the mock-up of a realistic scene used to assess DART-Lux SIF modeling. It is a 25 m x 25 m subzone (1 m x 1 m x 1 m voxels) of the C11 tree plot of the SERC forest that Yin et al. (2022) derived from airborne LiDAR measurements. Figure 3-7 compares the spectral nadir reflectance and also PSI and PSII radiance simulated by DART-FT and DART-Lux for 45 spectral bands from 400 to 850 nm. DART-Lux and DART-FT closely agree: relative difference is 1.15% for reflectance, 0.51% for PSI radiance and 0.40% for PSII radiance.

This simulation took 2 h 16 min and 4.8 GB of memory for DART-FT, 2 min 38 s and 1.5 GB for DART-Lux. It stresses the computational efficiency of DART-Lux for large and complex scenes.



Figure 3-6: 25 m x 25 m turbid mockup derived from LiDAR point cloud of SERC forest (USA) with pure green voxels (leaves or wood) and mixed brown voxels (leaves and wood).

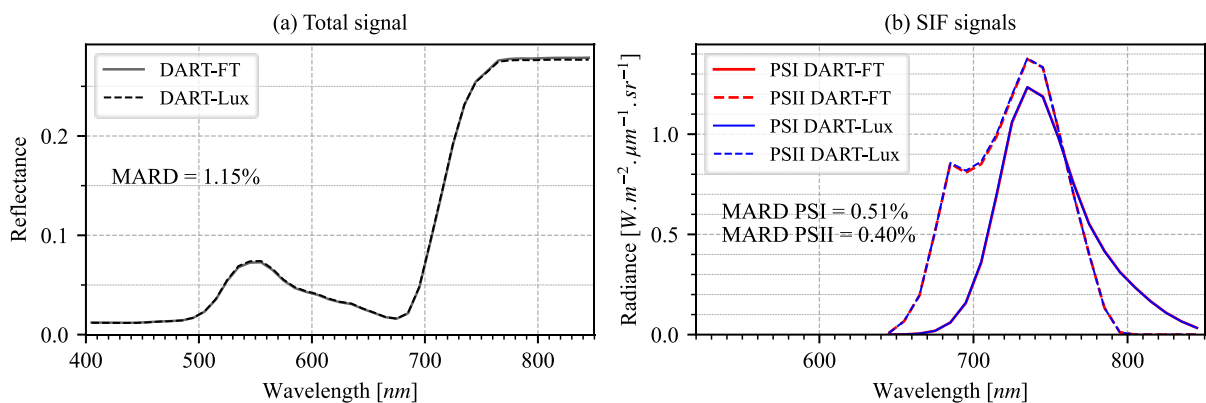


Figure 3-7: Nadir total reflectance and SIF radiance simulated using DART-FT (turbid) and DART-Lux (turbid) comparison

### 3.3 Conclusion

The theory of SIF emission modeling in DART-Lux has been introduced. It relies on major changes in DART-Lux. First, the SIF emission equations that include interdependence between spectral were adapted to the bi-directional path tracing algorithm and in particular to the sub-paths traced in the backward direction. Second, the turbid vegetation has been introduced, after having introduced fluid volumes using the double Henyey-Greenstein and the Rayleigh phase functions. DART-Lux now simulates SIF emission and observation for vegetation simulated as facets and/or as turbid volumes. It usually is much smaller simulation time and computer memory that DART-FT, with a gain in computational efficiency that depends on the scene complexity and on the number of simulated spectral bands. Therefore, it allows the study of much larger and more complex landscapes than DART-FT.

## Appendix 3-1: Inversion method

The inversion method is used to draw random samples from a random variable of a given PDF, using the inverse function of its CDF and a random number uniformly sampled over  $[0,1]$ .

Let a real random variable  $X$  with a PDF  $p_X(x)$  that we want to sample. The CDF of  $X$  is:

$$P_X(x) = p(X \leq x) = \int_{-\infty}^x p_X(t). dt$$

Let  $\Xi$  a random variable uniformly distributed over  $[0,1]$  and the random variable  $U=P_X^{-1}(\Xi)$ .

The PDF of  $\Xi$  is:  $p_{\Xi}(\xi) = \begin{cases} 1, & \text{if } \xi \in [0,1] \\ 0, & \text{otherwise} \end{cases}$

The CDF of  $\Xi$  is:  $P_{\Xi}(\xi) = \int_{-\infty}^{\xi} p_{\Xi}(t). dt = \begin{cases} 0, & \text{if } \xi < 0 \\ \xi, & \text{if } \xi \in [0,1] \\ 1, & \text{if } \xi > 1 \end{cases}$

Let us compute the CDF of the random variable  $U$ :

$$\begin{aligned} P_U(u) &= p(U \leq u) \\ &= p(P_X^{-1}(\Xi) \leq u) \\ &= p(\Xi \leq P_X(u)) \\ &= P_{\Xi}(P_X(u)) = P_X(u) \text{ (since } P_X(u) \in [0,1]) \end{aligned}$$

It implies that the random variable  $U=P_X^{-1}(\Xi)$  has the PDF of  $X$ :

$$p_U(u) = \frac{dP_U(u)}{du} = \frac{dP_X(u)}{du} = p_X(u)$$

Therefore, the random variable  $U$  can be used to draw samples of  $X$ .

## Appendix 3-2: Transmittance in hot spot configuration

For a turbid cell, transmittance in the hot spot configuration (Gastellu-Etchegorry et al., 1996) is:

$$Tr(\Omega_s, \Delta l) = \exp\left(-\int_{\Delta l} a(\Omega_s, \Omega_v, r). dr\right)$$

$$\text{with } a(\Omega_s, \Omega_v, r) = u_l \cdot G(\Omega_v) \cdot \left(1 - \sqrt{\frac{G(\Omega_s) \cdot |\mu_v|}{G(\Omega_v) \cdot |\mu_s|}} \cdot e^{-\frac{\Delta(\Omega_s, \Omega_v)}{s_f} \cdot r \cdot \mu_v}\right) = u_l \cdot G(\Omega_v) \cdot (1 - \beta \cdot e^{-\alpha \cdot r})$$

$$\text{Therefore: } Tr(\Omega_s, \Delta l) = e^{-u_l \cdot G(\Omega_v) \cdot [\Delta l + \frac{\beta}{\alpha} (e^{-\alpha \cdot \Delta l} - 1)]}$$

### Appendix 3-3: Studying the function $\phi(l)$

$$\phi(l) = l + \frac{\beta}{\alpha}(e^{-\alpha l} - 1), l \in \mathbb{R}$$

$$\phi'(l) = 1 - \beta \cdot e^{-\alpha l}$$

$$\phi'(l) = 0 \Leftrightarrow \beta \cdot e^{-\alpha l} = 1 \Leftrightarrow l = l_0 = \frac{\ln(\beta)}{\alpha}$$

$$\phi''(l) = \alpha \cdot \beta \cdot e^{-\alpha l} > 0 \Rightarrow \phi' \text{ is strictly increasing on } \mathbb{R}.$$

$\phi'(l_0) = 0$  implies  $\phi'(l) > 0 \forall l \in ]l_0, +\infty[$  and  $\phi'(l) < 0$  (i.e.,  $\phi$  strictly decreasing)  $\forall l \in ]-\infty, l_0[$

If  $l_0 > 0$  (i.e.,  $\beta > 1$ ), the equality  $\phi(0) = 0$  implies that  $\phi$  can be negative for  $l > 0$

$$\begin{aligned} \phi(l) = 0 &\Leftrightarrow l + \frac{\beta}{\alpha}(e^{-\alpha l} - 1) = 0 \Leftrightarrow l + \frac{\beta}{\alpha} \cdot e^{-\alpha l} - \frac{\beta}{\alpha} = 0 \\ &\Leftrightarrow l \cdot e^{\alpha l} + \frac{\beta}{\alpha} - \frac{\beta}{\alpha} \cdot e^{\alpha l} = 0 \\ &\Leftrightarrow l \cdot e^{\alpha l} - \frac{\beta}{\alpha} \cdot e^{\alpha l} = -\frac{\beta}{\alpha} \\ &\Leftrightarrow \alpha \cdot l \cdot e^{\alpha l} - \beta \cdot e^{\alpha l} = -\beta \\ &\Leftrightarrow (\alpha \cdot l - \beta) \cdot e^{\alpha l - \beta} = -\beta e^{-\beta} \\ &\Leftrightarrow \alpha \cdot l - \beta = W(-\beta e^{-\beta}) \\ &\Leftrightarrow \alpha \cdot l = W(-\beta e^{-\beta}) + \beta \end{aligned}$$

where  $W$  is “the Lambert W function” (Dence, 2013) defined as:  $z = x \cdot \exp(x) \Leftrightarrow x = W(z)$ . In the real domain,  $W$  has two branches:  $W_0$  and  $W_{-1}$  ( $W_0 \geq W_{-1}$ ). The branch  $W_0$  is used to have  $l \geq 0$

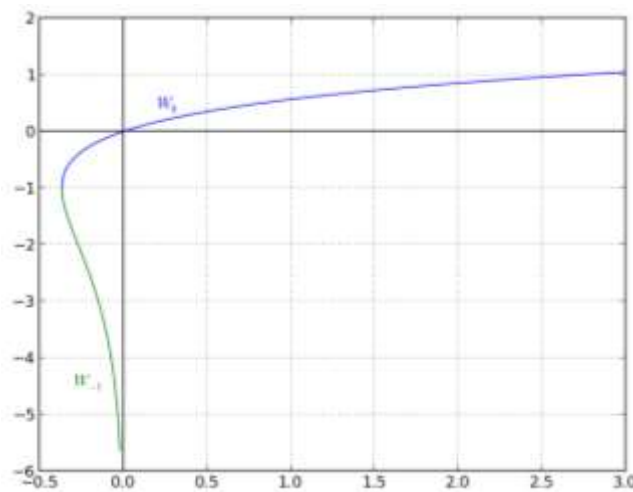


Figure 3-8: The  $W_0$  (blue) and  $W_{-1}$  (green) branches curves of the Lambert W function

$$\Leftrightarrow l = l_{w_0} = \frac{W_0(-\beta e^{-\beta}) + \beta}{\alpha} \text{ or } l = l_{w_{-1}} = \frac{W_{-1}(-\beta e^{-\beta}) + \beta}{\alpha}, (l_{w_0} > l_{w_{-1}})$$

If  $\beta \leq 1$ , then  $l_0 \leq 0$  and  $\phi$  strictly increasing on  $[0, +\infty[ \Rightarrow \phi$  bijective from  $[0, +\infty[$  to  $\phi([0, +\infty[) = [0, +\infty[$ . Otherwise, we can prove that  $l_{w_0} \geq l_0$ :

Then,  $\phi'(l) > 0, \forall l \in ]l_{w_0}, +\infty[$ . Hence,  $\phi$  is strictly increasing on  $]l_{w_0}, +\infty[$ .

Then,  $\phi$  is bijective from  $]l_{w_0}, +\infty[$  to  $\phi(]l_{w_0}, +\infty[) = [0, +\infty[$

Then for a sampled  $x = \phi(l) > 0$ ,  $\phi$  is bijective and we can find  $\phi^{-1}(x)$ .

Because  $W_0(-\beta e^{-\beta}) \geq -1$ , then:  $W_0(-\beta e^{-\beta}) + \beta \geq -1 + \beta$

Since  $-1 + \beta \geq \ln(\beta)$ , then  $W_0(-\beta e^{-\beta}) + \beta \geq \ln(\beta)$

Hence  $l_{w_0} \geq l_0 = \frac{\ln(\beta)}{\alpha}$

Computation of  $\phi^{-1}$

$$\begin{aligned} x = l + \frac{\beta}{\alpha}(e^{-\alpha l} - 1) &\Leftrightarrow x = l + \frac{\beta}{\alpha} \cdot e^{-\alpha l} - \frac{\beta}{\alpha} \\ &\Leftrightarrow x \cdot e^{\alpha l} = l \cdot e^{\alpha l} + \frac{\beta}{\alpha} - \frac{\beta}{\alpha} \cdot e^{\alpha l} \\ &\Leftrightarrow -\frac{\beta}{\alpha} = l \cdot e^{\alpha l} - \frac{\beta}{\alpha} \cdot e^{\alpha l} - x \cdot e^{\alpha l} \\ &\Leftrightarrow -\frac{\beta}{\alpha} = \left( l - \frac{\beta}{\alpha} - x \right) \cdot e^{\alpha l} \\ &\Leftrightarrow -\beta = (\alpha \cdot l - \beta - \alpha \cdot x) \cdot e^{\alpha l} \\ &\Leftrightarrow -\beta \cdot e^{-\alpha \cdot x - \beta} = (\alpha \cdot l - \beta - \alpha \cdot x) \cdot e^{\alpha \cdot l - \alpha \cdot x - \beta} \\ &\Leftrightarrow \alpha \cdot l - \alpha \cdot x - \beta = W(-\beta \cdot e^{-\alpha \cdot x - \beta}) \\ &\Leftrightarrow l = \frac{W(-\beta \cdot e^{-\alpha \cdot x - \beta}) + \alpha \cdot x + \beta}{\alpha} \end{aligned}$$

## Appendix 3-4: Sampling the Rayleigh phase function

The general form of the Rayleigh scattering phase function is

$$\frac{p(\theta)}{2\pi} = \frac{1}{4\pi} \cdot [A \cdot (1 + \cos^2(\theta)) + C]$$

It can be written as a function of  $\mu = \cos(\theta)$

$$p(\mu) = \frac{1}{2} \cdot [A \cdot (1 + \mu^2) + C] \quad \text{with } \int_{-1}^1 p(\mu) \cdot d\mu = 1$$

The CDF of  $p(\mu)$  is:  $P(x) = \int_{-1}^x p(\mu) \cdot d\mu$

$$\begin{aligned} &= \frac{1}{2} \int_{-1}^x [A \cdot (1 + \mu^2) + C] \cdot d\mu \\ &= \frac{1}{2} \left[ A \cdot \left( x + \frac{x^3}{3} + \frac{4}{3} \right) + C \cdot (x + 1) \right] \\ &= \frac{A}{6} \cdot x^3 + x \left( \frac{A}{2} + \frac{C}{2} \right) + \frac{2}{3}A + \frac{C}{2} \end{aligned}$$

To sample randomly a value  $\mu$  using a random number  $\xi \sim \mathcal{U}([0,1])$ :

$$\begin{aligned} P(\mu) = \xi &\Leftrightarrow \frac{A}{6} \cdot \mu^3 + \left( \frac{A}{2} + \frac{C}{2} \right) \mu + \frac{2}{3}A + \frac{C}{2} - \xi = 0 \\ &\Leftrightarrow \mu^3 + 3 \left( 1 + \frac{C}{A} \right) \mu - 2 \left( \frac{3\xi}{A} + \frac{3C}{2A} - 2 \right) = 0 \\ &\Leftrightarrow \mu^3 + 3\alpha\mu - 2\beta = 0 \quad \text{with } \alpha = 1 + \frac{C}{A}, \beta = \left( \frac{3}{A} \cdot \xi - \frac{3C}{2A} - 2 \right), \end{aligned}$$

This equation has a unique real solution:  $\mu = \left( \beta + \sqrt{\alpha^3 + \beta^2} \right)^{\frac{1}{3}} - \frac{\alpha}{\left( \beta + \sqrt{\alpha^3 + \beta^2} \right)^{\frac{1}{3}}}$

## Appendix 3-5: Nomenclature

Symbol	Description	Unit
$L(p' \rightarrow p)$	Radiance reaching $p$ from $p'$	$W \cdot m^{-2} \cdot \mu m^{-1} \cdot sr^{-1}$
$p_{\sigma_t}(l)$	Probability density function of having an interception at distance $l$	$m^{-1}$
$P_{\sigma_t}(l)$	Cumulated density function of $p_{\sigma_t}$	-



$Tr(\Delta l, \Omega_v)$	Path transmittance for a distance $\Delta l$ along the direction $\Omega_v$	-
$\sigma_a$	Absorption extinction coefficient	$m^2 \cdot m^{-3}$
$\sigma_s$	Scattering extinction coefficient	$m^2 \cdot m^{-3}$
$\sigma_t$	Total extinction coefficient	$m^2 \cdot m^{-3}$
$\Delta l$	Travel distance	$m$
$\Delta L$	Distance until the border of the volume	$m$

# Chapter 4

## Impact of vegetation 3D structure on SIF

1D SIF models are widely used for SIF studies. They might be appropriate to use for closed and homogeneous canopies with small leaves and no distinguishable rows, but they are much less appropriate for canopies with a strongly marked 3D structure. Section 2 of this chapter presents a study of the impact of vegetation 3D structure on SIF emission and observation over eight forest sites. This was done with a quasi-turbid representation of vegetation because DAT-Lux did not yet simulate turbid SIF modeling. This work was published in the Remote Sensing of Environment journal. Section 1 compares the quasi-turbid representation of vegetation to the turbid representation of vegetation.

### 4.1 Turbid versus quasi turbid modeling in DART-Lux

The study presented in section 4.2 was conducted before the introduction of turbid medium and SIF modeling with turbid medium in DART-Lux. Therefore, each turbid medium voxel was simulated as a voxel randomly filled by facets (*i.e.*, quasi-turbid medium) with the same leaf area as the turbid voxel. The quasi-turbid representation was created using the cloning capacity of DART-Lux in order to minimize the computer memory: each quasi-turbid voxel is a linear combination of a limited number of base 3D objects made as a random distribution of facets with a specific leaf area. Now that turbid modeling is available in DART-Lux, it is useful to

assess the validity of the quasi-turbid representation. The case study is the CI1 tree plot of the SERC forest (Regaieg et al., 2021) that Yin et al. (2022) derived by from airborne LiDAR point cloud. Its mean LAI value is  $5.517 \text{ m}^2 \cdot \text{m}^{-2}$  and its mean Wood Area Index value is  $0.792 \text{ m}^2 \cdot \text{m}^{-2}$ . The comparison is done without and with SIF simulation, for 45 spectral bands over  $[400,850\text{nm}]$  and a scene repetition equal to 1 (*i.e.*, the studied scene is surrounded by 8 identical scenes). The scattering phase function of the turbid medium is pre-computed for 200 discrete directions.

#### 4.1.1 No SIF simulation

Figure 4-1 shows the DART-Lux nadir reflectance of the CI1 tree plot simulated with the turbid and quasi-turbid representations, without SIF simulation. The quasi-turbid approximation shows a good accuracy with around 2% of relative difference.

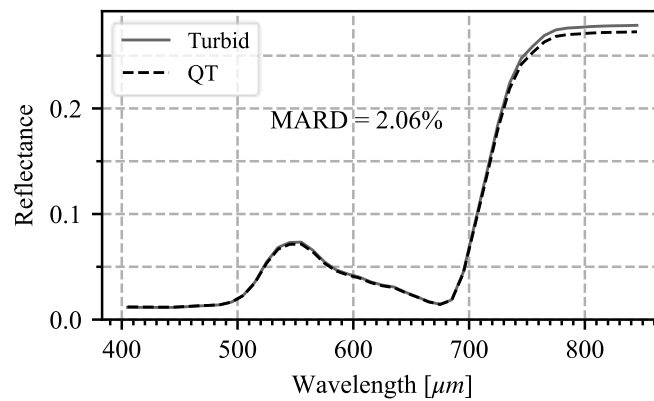


Figure 4-1: Nadir reflectance of the CI1 tree plot simulated as turbid and quasi-turbid (QT).

The Monte Carlo noise in DART-Lux images influences their pixel values. This is a constraint to be quantified. Here, it is done by running 10 times each simulation. Figure 4-2 shows the relative standard deviation images of the 10 runs averaged over all the spectral bands for the turbid and quasi-turbid representations. Each image is an average image of all spectral images of which each pixel value is the standard deviation of the 10 values from the 10 runs divided by the average of these 10 values. The relative standard deviation and therefore the Monte Carlo noise is lower for the turbid representation. This is mainly due to the fact that with, vegetation interaction is simulated using a single scattering phase function for a turbid representation, whereas for a quasi turbid medium, its simulation takes into account the discrete spatial and

## 4.1 TURBID VERSUS QUASI TURBID MODELING IN DART-LUX

angular distribution of individual leaves. For example, in order to mimick accurately the leaf angle distribution of the turbid medium, a very large number of leaves must be simulated.

Table 4-1 shows the comparison of the computation time and RAM requirements for the quasi-turbid and turbid simulations. The turbid simulation is slower than the quasi-turbid simulation, due to the use of computationally expensive operations such as the interpolation of phase function precomputed for a finite number of directions. On the other hand, it needs less RAM. Indeed, a turbid voxel is made of 12 facets (i.e., 2 triangles per voxel face) which is much less than the number of facets used to simulate a quasi turbid voxel.

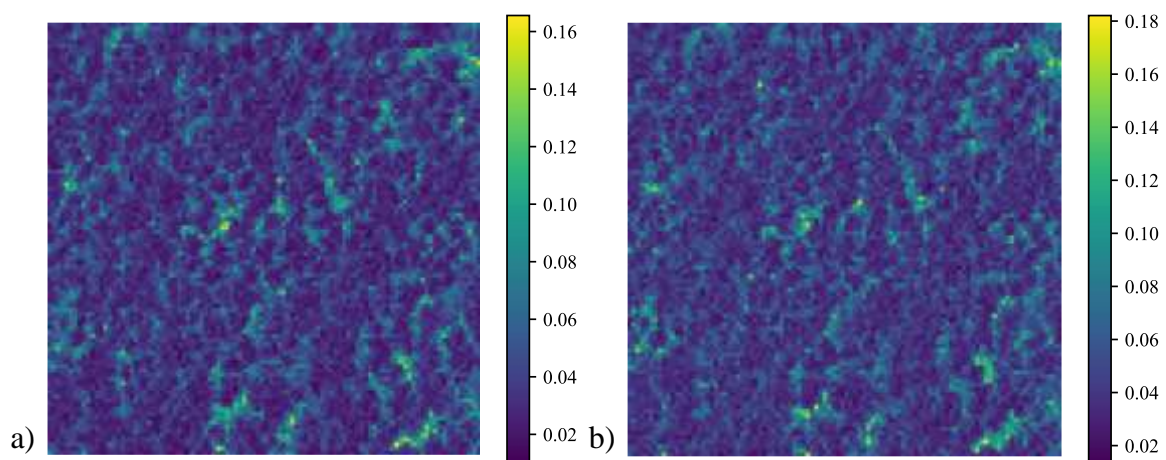


Figure 4-2: Relative standard deviation  $SD_r$  images averaged over all the spectral bands. a) Turbid medium (mean  $SD_r=0.0398$ ). b) Quasi turbid medium (mean  $SD_r=0.0475$ ).

Table 4-1: Computational needs for quasi-turbid and turbid DART-Lux simulations.

	Quasi-Turbid	Turbid
Computation Time	15 min	36 min
RAM	13.1 GB	5.2 GB

### 4.1.2 With SIF simulation

Figure 4-3 shows the canopy nadir PSI and PSII radiance for the turbid and quasi-turbid representations. The order of magnitude of the relative difference between the two representations is the same as if the SIF is not simulated (Figure 4-1).

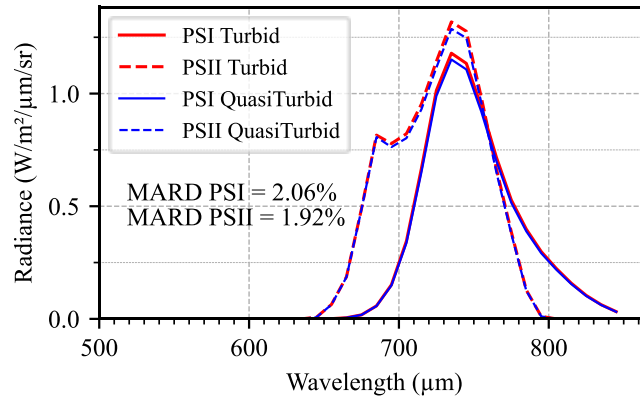


Figure 4-3: PSI and PSII radiance of CI1 tree plot for the turbid and quasi-turbid representations.

Figure 4-4 shows the relative standard deviation images of 10 runs averaged over all the spectral bands for turbid-and quasi turbid simulations, for PSI and PSII SIF radiance. As for the total signal, the Monte Carlo noise for SIF is higher for the quasi-turbid representation.

Table 4-2 shows the computation time and RAM requirements for quasi-turbid and turbid SIF simulations. The increase factor of computation time between quasi-turbid and turbid is higher if SIF is simulated. Indeed, the interpolation on the SIF transfer functions ( $N \times N$  matrices for  $N$  spectral bands) is more computationally expensive than the interpolation of normal scattering phase functions ( $N$ -element vector for  $N$  spectral bands).

The RAM requirements is nearly the same for quasi-turbid no SIF and SIF simulations, while, it is larger for the turbid SIF compared to the turbid with no SIF because the SIF transfer functions computed for all incident and outgoing directions, and also excitation and emission bands, for PSI and PSII, can be voluminous. However, in this case, the RAM requirement is still less than for the quasi-turbid simulation.

This work stresses that depending on configurations (*i.e.*, number of spectral bands, dimension of the study area, etc.), the quasi turbid or the turbid representation can be preferred.

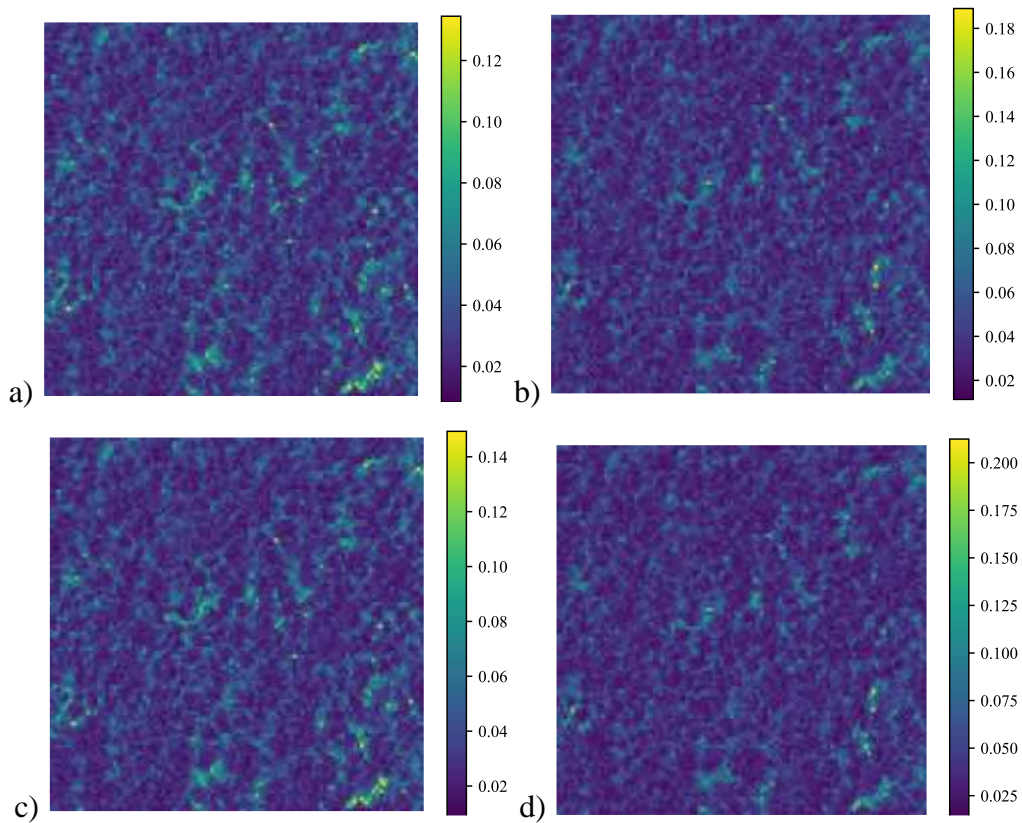


Figure 4-4: Relative standard deviation images for SIF averaged over the spectral bands where it is non null. a) PSI turbid (average = 0.0327) b) PSI quasi-turbid (average = 0.0412) c) PSII turbid (average = 0.0341) d) PSII quasi-turbid (average = 0.0430).

Table 4-2: Computational requirements for quasi-turbid and turbid SIF simulations

	Quasi-Turbid	Turbid
Computation Time	1 h 25 min	5 h 25 min
RAM	13.1 GB	8.1 GB

## 4.2 Article

The use of 1D SIF models like SCOPE implies to use a less accurate representation of vegetation as horizontally homogeneous layers and to neglect the 3D structure of canopies although it highly impacts the propagation of light and SIF radiation with the canopy. It neglects

## *CHAPTER 4: IMPACT OF VEGETATION 3D STRUCTURE ON SIF*

other important elements of the canopy as well, that interact with radiation and influence the SIF emission and the measured signal such as the local topography and the woody elements of the trees. Hence, the use of 1D models can induce errors in SIF simulations and consequently errors in the interpretation of SIF measurements. Therefore, it is important to study the impact of 3D structure on the SIF and to quantify the simulation errors that are made when simulating the SIF with 1D models. Consequently, 3D radiative transfer models are more accurate. In addition, a 3D models like DART can simulate the SIF for any 1D and 3D representation of vegetation, which is very useful for many studies.

This study was conducted on eight realistic 3D mock-ups derived by inversion of airborne LiDAR measurements over the SERC forest (Yin et al., 2022). It allowed one to stress that compared to 3D representations, 1D representations can lead to very large errors on PAR absorption, SIF emission, and SIF radiance from morning to evening, depending on the landscape 3D architecture. In this work, the order of magnitude of errors was often larger than 30%. This work was published in *Remote Sensing of Environment* (Regaieg et al., 2021).





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## Assessing impacts of canopy 3D structure on chlorophyll fluorescence radiance and radiative budget of deciduous forest stands using DART

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## ABSTRACT

Although remote sensing (RS) of solar-induced chlorophyll fluorescence (SIF) is increasingly used as a valuable source of information about vegetation photosynthetic activity, the RS SIF observations are significantly influenced by canopy-specific structural features (i.e., canopy architecture including leaf area index and presence of woody components), atmospheric conditions during their acquisition (e.g., proportion of direct and diffuse irradiance) and observational geometric configurations (e.g., sun and viewing directions). Radiative transfer (RT) models have the potential to provide a better understanding of the canopy structural effects on the SIF emission and RS signals. Here, we used the DART model to assess the daily influence, from morning to evening, of forest 3D architecture on SIF nadir radiance, emission, escape factor and nadir yield of eight 100 m × 100 m forest study plots established in a temperate deciduous forest of the Smithsonian Environmental Research Center (Edgewater, MD, USA). The 3D architecture of each plot was derived from airborne LiDAR. DART simulations of these 3D forest plots and their 1D (i.e., vertical profile of sun-adapted and shade-adapted leaves) and 0D (i.e., homogeneous layer of sun-adapted leaves above an homogeneous layer of shade-adapted leaves) abstractions were compared to assess the relative errors ( $\epsilon_{1D-3D}$  and  $\epsilon_{0D-3D}$ ) associated with horizontal and vertical structural heterogeneity, respectively. Forest 3D structure, especially horizontal heterogeneity, had a great influence on forest nadir SIF radiance, resulting in  $\epsilon_{1D-3D}$  up to 55% at 8:00 and 18:00 (i.e., for oblique sun directions). The key indicators of this impact, in the descending order of importance, were the SIF escape factor ( $\epsilon_{1D-3D}$  up to 40%), the attenuation of incident photosynthetically active radiation ( $\epsilon_{1D-3D}$  less than 5%), and the SIF emission yield ( $\epsilon_{1D-3D}$  less than 2%). The influence of forest architecture on the nadir SIF escape factor and SIF yield ( $\epsilon_{1D-3D}$  up to 40%) varied over time, with differences in forest stand structure, and per spectral domain, being always larger between 640 and 700 nm than between 700 and 850 nm. In addition, woody elements demonstrated a large influence on forest SIF radiance due to their “shading” effect ( $\epsilon$  up to 17%) and their “blocking” effect ( $\epsilon \approx 10\%$ ), both of them higher for far-red than for red SIF. These results underline the importance of 3D forest canopy architecture, especially 2D heterogeneity, and inclusion of woody elements in RT modeling used for interpretation of the RS SIF signal, and subsequently for the estimation of gross primary production and detection of vegetation stress.

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1        **1. Introduction**

2        Solar-induced chlorophyll fluorescence (SIF) is a photoprotective electromagnetic radiation  
3        emitted by chlorophyll molecules in response to absorption of photosynthetically active  
4        radiation (PAR) by green vegetation. Since the energy emitted as SIF is complementary to the  
5        energy entering the photochemical processes and the excessive energy dissipated as heat (Baker,  
6        2008; Mohammed et al., 2019), it is considered as an indicator of the functional state of plant  
7        photosynthesis (Baker, 2008). SIF measurements are complicated by the fact that SIF represents  
8        only a small fraction of absorbed PAR and spectrally overlaps with radiation reflected by Earth  
9        surface elements and the atmosphere. However, the improvement of remote sensing (RS)  
10       optical sensors and techniques for retrieving the SIF signal (Meroni et al., 2009; Mohammed et  
11       al., 2019) has opened new avenues for monitoring the functional state of vegetation. SIF can be  
12       used to track actual photosynthetic efficiency (Rossini et al., 2015; Campbell et al., 2019; Yang  
13       et al., 2021), to improve assessment of plant gross primary production (Guanter et al., 2014; Z.  
14       Liu et al., 2019), and to detect vegetation stress (Ač et al., 2015). This diverse potential of SIF  
15       for vegetation monitoring spurred the development of methods for space-borne measurements  
16       and new satellite missions, such as the FLuorescence EXplorer (FLEX) selected by the  
17       European Space Agency (ESA) as its 8<sup>th</sup> Earth explorer scientific mission (Drusch et al., 2017).  
18       Besides plant photosynthetic activity, SIF observations are impacted by other confounding  
19       factors, notably the structure of vegetation canopies (Fournier et al., 2012; Migliavacca et al.,  
20       2017) and PAR availability. They are of SIF also influenced by sun-canopy-sensor angular and  
21       directional effects (Zhang, Zhang, Porcar-Castell, et al., 2020; Zhang, Zhang, Zhang, et al.,  
22       2020), and are driven by wavelength-dependent phenomena of SIF emission, scattering, and re-  
23       absorption. For instance, Fournier et al. (2012) found that the red-to-far-red fluorescence ratio  
24       could decrease by a factor of two between the leaf level and the canopy level, due to a higher  
25       absorption of red SIF by the vegetation canopy. Therefore, accurate interpretation and use of  
26       SIF RS observations require understanding of three consecutive processes: i) interception of  
27       photosynthetically active radiation (PAR; 400 - 750 nm) and its absorption by foliar elements  
28       ( $APAR_{green}$ ;  $W.m^{-2}$ ), due to chlorophyll pigments in leaves, ii) leaf SIF emission from  
29       photosystems I and II (PSI and PSII) in thylakoid membranes, due to  $APAR_{green}$ , and iii)  
30       propagation of the SIF radiation through the canopy, including its scattering and absorption by  
31       different canopy elements, *i.e.*, leaves, woody elements, litter, bare soil, and others (van der Tol  
32       et al., 2019).

33 Radiative transfer models (RTMs) are powerful tools used for various vegetation RS  
34 applications, ranging from sensitivity analyses (Malenovský et al., 2008) to quantitative  
35 retrievals of models' biophysical inputs (Brede et al., 2020; Verrelst et al., 2019). The  
36 increasing need for understanding and interpreting the SIF signal at canopy level resulted in  
37 coupling canopy RTMs with a leaf-level SIF model, most frequently with Fluspect (Vilfan et  
38 al., 2016). The pioneer in one-dimensional (1D) SIF canopy modeling is SCOPE (van der Tol  
39 et al., 2009). Based on SAIL RTM (Verhoef, 1984) and coupled with leaf-level SIF and  
40 biochemistry models, SCOPE models photosynthesis and the full energy balance (Damm et al.,  
41 2015; Migliavacca et al., 2017; Verrelst et al., 2015, 2016). Despite its extension to vertically  
42 heterogeneous canopies (Yang et al., 2017), SCOPE's 1D formulation makes it less suitable for  
43 structurally complex and spatially heterogeneous canopies, such as forests. This explains the  
44 recent development of three-dimensional (3D) SIF RTMs, such as FluorFLIGHT (Hernández-  
45 Clemente et al., 2017), based on the 3D FLIGHT model (North, 1996), FLiES-SIF (Sakai et al.,  
46 2020) based on the FLiES model (Kobayashi & Iwabuchi, 2008) that simulate SIF for tree  
47 canopies, FluorWPS (Zhao et al., 2016) based on the WPS model (Zhao et al., 2015) designed  
48 to simulate SIF of structurally complex canopies and the FluLCVRT model (Kallel, 2020) that  
49 simulates SIF for 3D canopies including 3D leaf-level SIF modeling. The work presented in  
50 this paper was carried out with the 3D discrete anisotropic radiative transfer (DART) model  
51 (Gastellu-Etchegorry et al., 2017) coupled with Fluspect-Cx (Vilfan et al., 2018). DART  
52 simulates both the 3D SIF radiative budget (*i.e.*, interception, absorption, emission and  
53 scattering) and the SIF signal remotely sensed at the bottom of atmosphere (BOA) and top of  
54 atmosphere (TOA) for forest or crop canopies. It upscales leaf-level SIF to canopy SIF, while  
55 considering the user-defined leaf biochemistry and fluorescence quantum yield efficiencies of  
56 PSI and PSII, and accounting for the actual 3D vegetation architecture. DART has been cross  
57 compared with the SCOPE modeling of the same 1D vegetation scenarios (Malenovský et al.,  
58 2021), and used in various studies for sensitivity analyses of the SIF signal in architecturally  
59 complex forest canopies (W. Liu et al., 2019; Malenovský et al., 2021), scaling canopy-level  
60 SIF down to the level of photosystems (X. Liu et al., 2019), and studying the escape probability  
61 of far-red SIF from discontinuous forest canopies (W. Liu et al., 2020).

62 The main objective of this paper is to assess the impact of temperate deciduous forest  
63 architecture on the diurnal variability in the nadir SIF RS signal and within-canopy SIF  
64 emission by green leaves. SIF canopy signals were simulated with a new Monte Carlo mode of

65 DART, called DART-Lux, whereas the radiative budget of within canopy SIF emission was  
66 simulated using the standard flux tracking mode of DART, called DART-FT. (cf. section 2.1).

## 67 **2. Material and methods**

### 68 **2.1. Discrete anisotropic radiative transfer (DART) modeling approaches**

69 DART (<https://dart.omp.eu>) is a comprehensive physically based 3D RTM developed by the  
70 CESBIO Laboratory (Toulouse, France) since 1993 (Gastellu-Etchegorry et al., 1996, 2015). It  
71 is continuously improved both scientifically (*e.g.*, light polarization and radiative coupling  
72 between the atmosphere and Earth surfaces) and technically (*e.g.*, computational efficiency in  
73 terms of simulation time and computer memory). It simulates the radiative budget (RB) as well  
74 as TOA, BOA, and in-situ RS observations (*i.e.*, LiDAR and imaging spectroradiometer data,  
75 either pushbroom scanner, hemispherical or frame camera) of urban and natural landscapes  
76 from the visible to the thermal infrared spectral domains, for any experimental and instrumental  
77 configuration (solar illumination, viewing direction, atmosphere condition, spatial and spectral  
78 resolutions, etc.). DART is made of three radiative transfer modeling modules:

- 79 1. DART-FT (Flux Tracking) simulates passive optical RS signals and 3D RB, including SIF,  
80 using an adaptation of the N-flux discrete ordinates' method (Yin et al., 2013, 2015).  
81 Landscapes are simulated as the juxtaposition of planar triangular facets in 3D arrays of  
82 voxels that contain fluid and turbid medium (*i.e.*, vegetation volume statistically  
83 characterized by a leaf angular distribution (LAD) and a leaf area index (LAI) equivalent  
84 to a volume filled with an infinite number of infinitely small planar surfaces).
- 85 2. DART-RC (Ray Carlo) combines Monte Carlo (MC) and FT methods in order to simulate  
86 LiDAR signals (Gastellu-Etchegorry et al., 2016; Yin et al., 2016). 3D landscapes are  
87 simulated in the same way as for DART-FT module.
- 88 3. DART-Lux is a new module that broadens the application domain of DART to large  
89 landscapes through the introduction of a bidirectional MC modeling approach adapted from  
90 the physically based and unbiased rendering engine called LuxCoreRender (Georgiev et  
91 al., 2012; *LuxCoreRender – Open Source Physically Based Renderer*). It greatly improves  
92 the computational efficiency of simulations for large and complex landscapes. For example,  
93 the reduction of simulation time and computer memory can be over 100-times. Indeed, this  
94 DART mode only tracks radiation that impacts the signal forming the sensor observation.

95 Landscapes are simulated as the juxtaposition of facets and volumes filled with fluids and  
96 turbid medium. Volumes in DART-Lux can be defined independently from the 3D arrays  
97 of voxels, unlike DART-FT and RC. Although still under intensive testing, DART-Lux  
98 already simulates most RS products of DART-FT and DART-RC, including SIF and  
99 LiDAR. Presently, TOA signals are simulated using DART-FT based atmosphere  
100 modeling (Wang & Gastellu-Etchegorry, 2021). MC-based modeling of atmosphere  
101 thermal radiative transfer, as well as radiative budget are under development.  
102

103 SIF modeling was initially introduced in DART-FT for vegetation canopies represented explicitly  
104 with facets (Gastellu-Etchegorry et al., 2017) and later for canopies simulated with 3D turbid  
105 voxels (Regaieg et al., 2020). More recently, SIF modeling was also implemented in DART-Lux,  
106 for both facet-based as well as turbid canopies (Regaieg et al., in preparation). As indicated above,  
107 compared to the standard DART-FT mode, DART-Lux is much more efficient in terms of  
108 computation time and required memory to simulate RS images, including SIF images. However,  
109 up to now it does not simulate the landscape RB. Therefore, in this work, we simulated SIF image  
110 observations at the spatial resolution of 1m in DART-Lux, whereas the forest RB was simulated  
111 in DART-FT at a lower spectral resolution to reduce computational demand.

112 The leaf radiative transfer model Fluspect-Cx, which was embedded in DART and tested by  
113 (Malenovsky et al., 2021), simulates additionally to leaf spectral reflectance and transmittance  
114 optical properties the forward and backward fluorescence excitation-emission matrices per  
115 photosystem (PSI and PSII). Its inputs include contents of foliar pigments, water and dry matter,  
116 a structural parameter characterizing the leaf optical thickness, and leaf fluorescence quantum  
117 efficiencies  $fqe$  (*i.e.*, fraction of  $APAR_{green}$  emitted as fluorescence) of a dark-adapted leaf, that  
118 are in DART referred to as PSI and PSII fluorescence yields. Leaf physiology and local  
119 climatology influence  $fqe$ . However, unlike the SCOPE model, DART does not contain a leaf  
120 biochemical model, and therefore cannot simulate the canopy climatic weights that condition leaf  
121  $fqe$ . Therefore, in DART,  $fqe$  is an input parameter that can be specified per individual foliage  
122 facet, per group of foliage facets, per type of turbid medium, or as a single value for all leaf  
123 facets and turbid medium types. Groups of foliage facets can correspond, for instance, to sunlit  
124 and shaded leaves (*i.e.*, leaves irradiated by direct sun or not at a certain time), or to sun- and  
125 shade-adapted leaves (*i.e.*, leaves that have grown under and adapted to high or low light  
126 intensity such that biochemical contents vary), knowing that a sun-adapted leaf can be

127 momentarily a shaded leaf and vice versa. In this work, forest *fqe* values published in (W. Liu  
 128 et al., 2019) are used. Although very likely differing from actual values of the study forest sites,  
 129 these values are sufficiently representative to investigate the impact of forest architecture and  
 130 different structures (*e.g.*, wood components) on canopy SIF signal and emission. We also note  
 131 that although sun-adapted and shade-adapted *fqe*'s are considered, the actual light and temperature  
 132 modulations are not. Consequently, a leaf emitted SIF is given by APAR and *fqe* per leaf  
 133 adaptation.

134

## 135 2.2. Study sites

136 Eight deciduous forest sites in the Smithsonian Environmental Research Center (SERC,  
 137 Edgewater, MD, USA) were selected as the study sites. The stands mainly consist of mixed-  
 138 species deciduous forests of *Liquidambar styraciflua* and *Liriodendron tulipifera* for the  
 139 overstory, and *C. tomentosa*, *Quercus alba*, and *F. grandifolia* for the understory (Kamoske et  
 140 al., 2019; Parker, 1995). Descriptions of forest stands and management characteristics can be  
 141 found in (Brush et al., 1980, Parker et al., 2001, McMahon et al., 2010). Four forest stand types  
 142 were selected from the combinations of both canopy development categories [“intermediate”  
 143 (I) or “mature” (M)] and experimental status categories [“control” (C) or “logged” (L)], and  
 144 two sites of each type (indexed 1 and 2) were used for this study (Table 1). Therefore, the eight  
 145 study sites (Figure 1) have different canopy architectures, as illustrated by their height maps  
 146 (Figure 2) and LAI vertical profiles. The forest plots LI2, LM1, LM2, and, to a lesser extent,  
 147 LI2, have a larger horizontal heterogeneity than the other plots. These plots also have  
 148 pronounced heterogeneity, with foliage density being larger (*i.e.*, larger LAI voxel values in  
 149 DART-FT) in the bottom canopy layers than in the top canopy layers. Table 2 shows the wood  
 150 area density and the LAI for sun- and shade-adapted leaves (*cf.* Section III-1). We note that the  
 151 concept of wood area density does not have an actual physical meaning linking with trunks and  
 152 branches’ surface areas. It is derived from leaf off G-LiHT ALS data, and used to compensate  
 153 the interception contribution induced by woody part. The presence of a local topography  
 154 explains why the total ground area (*i.e.*, area based on DEM; Table 2) is larger than the scene  
 155 area (*i.e.*,  $100\text{ m} \times 100\text{ m}$ ). Leaf chlorophyll a+b and carotenoid contents ( $\mu\text{g cm}^{-2}$ ) were  
 156 derived from top of canopy leaf samples collected at SERC in July of 2017 (Campbell et al.,  
 157 2018), and measured using established protocol described in (Campbell et al., 2007). Pigments  
 158 were extracted in dimethyl sulfoxide, identified spectro-photometrically at 1-nm resolution

159 using a dual-beam spectrophotometer (Perkin-Elmer; Wellesley, MA, USA) and calculated  
 160 using absorption coefficients and equations described by (Wellburn, 1994).

161 Biochemical and optical properties of leaves, woody elements and soil properties used in DART  
 162 are listed in Table 3. The overall LAI of 3-D reconstruction has been validated against field  
 163 litter-collection measurements in 2012 for various voxel dimensions from 0.5m to 5m.

164

165 Table 1. Study sites' nomenclature and description.

	Abbreviations	Description
Experimental status categories	C (Control)	No known management
	L (Logged)	Selective harvest (~ 50% of basal area)
Canopy development categories	M (Mature)	~125 years-old at time of harvesting
	I (Intermediate)	~70 years old at time of harvesting

166

167 Table 2. Wood area density, LAI (per sun-/shade-adapted leaves) and DEM-derived area for each site.

Parameter/Study site	CI1	CI2	CM1	CM2	LI1	LI2	LM1	LM2
Wood area density ( $m^2 \cdot m^{-2}$ )	0.792	0.863	0.939	0.991	0.665	0.435	0.827	0.615
Sun-adapted LAI ( $m^2 \cdot m^{-2}$ )	2.916	3.093	3.697	3.160	1.964	0.951	1.341	1.920
Shade-adapted LAI ( $m^2 \cdot m^{-2}$ )	2.601	2.847	2.996	3.174	3.181	2.810	3.419	3.559
Area based on DEM ( $m^2$ )	12450.7	14475.9	16535.3	11297.9	17628.8	15395.0	17576.3	20142.0

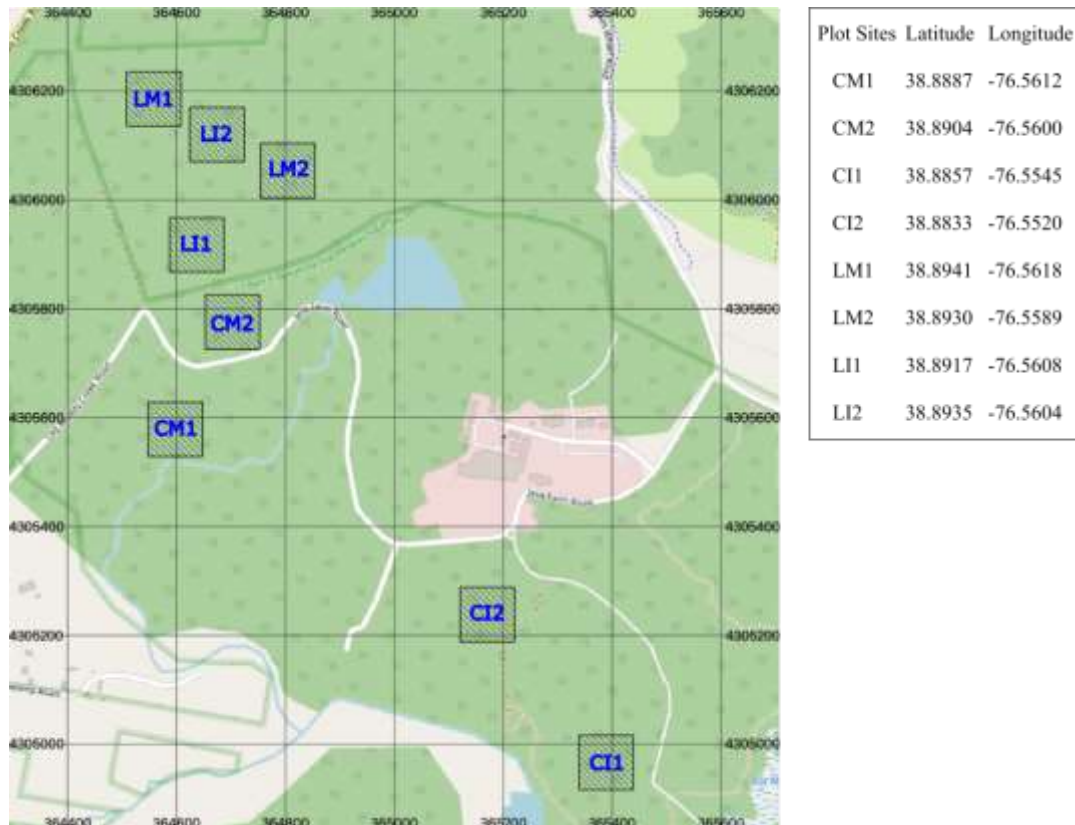
168

169

Table 3. Biochemical and optical properties used in DART modeling of the study sites.

Parameter/Study site	CI1	CI2	CM1	CM2	LI1	LI2	LM1	LM2
Leaf chlorophyll a+b content ( $\mu g. cm^{-2}$ )	24.307	23.253	20.23	18.146	20.569	23.264	19.619	20.165
Leaf total carotenoid content ( $\mu g. cm^{-2}$ )	7.06	6.81	6.338	5.852	6.295	6.843	6.156	6.364
Leaf dry matter content ( $g. cm^{-2}$ )	0.012							
Leaf equivalent water thickness (cm)	0.009							
Leaf fluorescence quantum efficiency	PSI: 0.0053, PSII: shade-adapted: 0.0201, sun-adapted: 0.0154							
Wood optical property	Bark of <i>Populus tremuloides</i>							
Soil optical property	Loam-gravelly brown dark soil (Alfisol from the spectra library: <a href="http://speclib.jpl.nasa.gov/">http://speclib.jpl.nasa.gov/</a> )							

170



171

172 Figure 1. Locations of SERC forest study sites (Edgewater, MD, USA) and G-LiHT flight paths.

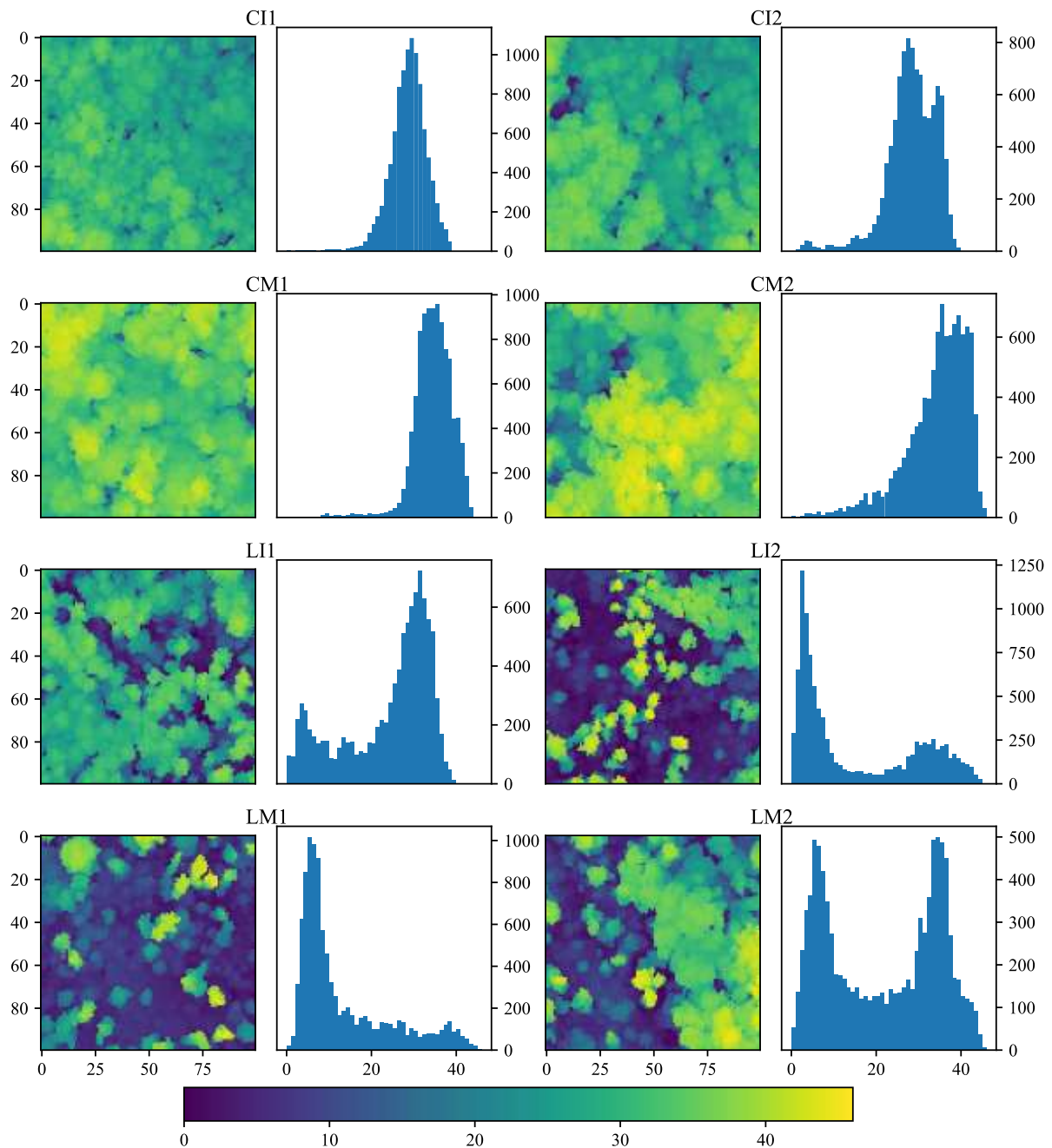
173

### 174 2.3. Creation of 3D forest abstractions from airborne LiDAR acquisitions

175 The 3D abstractions (mock-ups) of the eight forest sites were derived from 2012 multi-  
 176 directional and multi-temporal acquisitions by an airborne discrete-return LiDAR scanner  
 177 (Riegl's VQ480i), which is part of the Goddard's LiDAR, Hyperspectral and Thermal (G-LiHT)  
 178 Airborne Imager (Cook et al., 2013). The LiDAR acquisitions were taken during two forest  
 179 growth stages: i) the leaf-off stage (in March) and ii) the leaf-on stage (in June). Each  
 180 constructed forest mock-up ( $100m \times 100m$ ) corresponds to a 3D array of  $1m$ -size voxels filled  
 181 with a turbid medium. The leaf angle distribution varies with height following an ellipsoidal  
 182 distribution generated by mean leaf incline angle from  $10^\circ$  at the lower canopy to  $60^\circ$  at the  
 183 upper canopy. In this experiment, we assumed an overall leaf incline angle of  $57.3^\circ$  over the  
 184 whole canopy, which may induce a slight underestimation of LAI at the upper canopy and over  
 185 estimation at the lower canopy in scene construction. This assumption has minor influence since  
 186 the change of incline angle is correlated with sun illumination, where majority of the sunlight  
 187 is intercepted by the leaves with larger incline angle. Since the objective was to investigate



188 changes in the diurnal variation of canopy SIF radiance and leaf emissions on 15 June 2017  
 189 between 7.00 and 19.00 (local time, with a time step of 1 h), the DART simulated solar zenith  
 190 angles (SZA) and solar azimuth angles (SAA) were adjusted accordingly, with for example  
 191 (SZA, SAA) = (76.85°, 109.51°) at 7.00, (15.62°, 5.8°) at 13.00, and (74.33°, 252.4°) at 19.00  
 192 of the local time.



193

194 Figure 2. Maps and histograms of forest top-of-canopy height (m) for the eight forest study sites.

195

196 Table 4. Forest plot mean height and height standard deviation and number of pure bare ground pixels.

Plot	CI1	CI2	CM1	CM2	LI1	LI2	LM1	LM2
Mean Height (m)	28.65	28.34	34.54	34.33	23.80	15.19	13.31	21.75
Height standard deviation (m)	4.37	5.90	4.61	7.32	10.44	14.03	10.88	13.17
Number of pure bare ground pixels (out of 10 000)	2	1	2	4	89	258	8	48

197

198 **2.4. Preprocessing of modeled forest scenes**

199 Leaf biochemical and anatomical properties are adapted to the leaf exposure to sun direct and  
200 scattered diffuse radiation (Givnish, 1988; Nobel, 1976). To assess 3D distribution of sun- and  
201 shade-adapted foliage in each forest plot, we used DART-FT to compute hourly time series of  
202 3D RB in the PAR domain from sunrise to sunset on 15 June 2012, with SZA and SAA as  
203 specified in the section 2.3. The diurnal radiation intercepted by foliar elements in each turbid  
204 voxel of the 3D plots computed by DART-FT was then used to classify the foliage turbid voxels  
205 of each forest plot into sun- and shade-adapted foliage voxel groups. Sun- and shade-adapted leaf  
206 classification methods based on thresholds on the intercepted radiation were developed for the  
207 DART model for vegetation canopies simulated as facets (Malenovský et al., 2021). Here, in the  
208 absence of information on the threshold definition, and for a vegetation canopy simulated as  
209 turbid voxels, we chose to simply define classification decision threshold in such a way that the  
210 numbers of sun-adapted voxels and shade-adapted voxels were equal. Subsequently, specific *fqe*  
211 input values were assigned to the sun-adapted and shade-adapted cells (W. Liu et al., 2019)

212 Since the DART-FT mode was slow and too demanding for computer memory when simulating  
213 SIF radiance of the forest plots represented by many voxels ( $>10^5$ ) for 372 spectral bands (Table  
214 5), we used the DART-Lux mode instead. As DART-Lux could at that time only simulate the  
215 SIF signal of landscapes represented by geometrical facets, a “turbid-to-facet” conversion  
216 procedure was designed to transform the forest turbid mock-ups (already classified into sun-  
217 adapted and shade-adapted voxels) into forest 3D abstractions with leaf and woody elements  
218 being represented with solid facets (cf. Appendix). DART-FT and DART-Lux give nearly  
219 equivalent results in terms of canopy reflectance and SIF radiance (cf. Appendix). Small  
220 differences may be observed due to the different strategies adopted by the two modes (*i.e.*,  
221 discrete ordinates for DART-FT, Bi-directional Monte Carlo for DART-Lux), and also due to

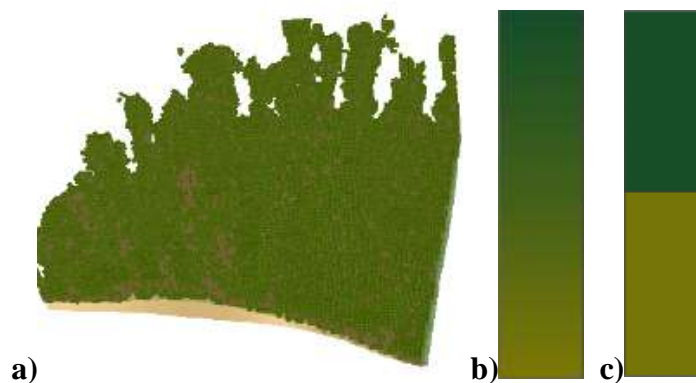
222 the approximation of turbid volumes by clouds of facets. These differences are supposed to be  
 223 negligible compared to the differences caused by the canopy structure.

224 **2.5. Simulated structural complexity**

225 Three structurally different forest abstractions were considered for this study (Figure 3):

- 226 1. 3D mock-ups: derived from airborne LiDAR data, with classified sun- and shade-adapted  
 227 cells as explained in the two previous sections.
- 228 2. 1D mock-ups: horizontally homogenized 3D mock-ups having the same heights and vertical  
 229 profiles of sun- and shade-adapted leaf area density and wood area density but missing the  
 230 forest horizontal heterogeneity.
- 231 3. 0D mock-ups: horizontally and vertically homogenized mock-ups having the mean height  
 232 of the original 3D canopies, shade-adapted leaves homogeneously distributed in the mock-  
 233 up bottom half, sun-adapted leaves homogeneously distributed in the mock-up top half, and  
 234 woody elements homogeneously distributed within the entire scene. Compared to 3D forest  
 235 mock-ups, 0D mock-ups miss the forest horizontal and vertical heterogeneity, including the  
 236 simplifying assumption that all sun-adapted leaves are located at the top and all the shade-  
 237 adapted leaves are located at the bottom of the canopy.

238



239

240 Figure 3: The three types of scene abstractions: a) 3D, b) 1D, c) 0D (top: sun-adapted, bottom: shade-  
 241 adapted leaves)

242

243 **2.6. Simulated SIF products**

244 SIF nadir images of a high spectral resolution, from 0.15 nm to 4 nm (Table 5), were simulated  
 245 with DART-Lux. DART-FT was used to simulate the PAR and SIF radiative budget with a

246 lower spectral resolution ([400-640 nm] at 20 nm resolution, [640-850] at 10 nm resolution)  
 247 and 40 discrete directions, in order to limit computational demands.

248

249 Table 5. The 372 spectral bands of DART-Lux simulations. They over-sample the O<sub>2</sub>B (~687nm) and  
 250 O<sub>2</sub>A (~760nm) oxygen absorption bands, and under-sample the [400-640nm] band (no SIF emission)

Spectral interval (nm)	Spectral resolution (nm)	Number of spectral bands
400-640	4	60
640-641.5	1.5	1
641.5-686.5	1	45
686.5-694	0.15	50
694-694.5	0.5	1
694.5-759.5	1	65
759.5-770	0.15	70
770-770.5	0.5	1
770.5-848.5	1	78
848.5-850	1.5	1

251

252 The influence of the canopy 3D architectures on 3D SIF emissions was assessed by comparing  
 253 the DART-FT RB fluxes (*i.e.*, intercepted, scattered, absorbed and emitted PAR and total SIF  
 254 radiation) per voxel in the simulated 3D, 1D and 0D mock-ups. Here, the PAR absorbed by  
 255 leaves (W.m<sup>-2</sup>) informs us on APAR<sub>green</sub> (the 1<sup>st</sup> process). SIF<sub>emitted</sub> (W.m<sup>-2</sup>) is the sum of PSI  
 256 and PSII emissions by adaxial and abaxial sides of all leaves in the canopy. It depends on the  
 257 directionality and intensity of the incident PAR relative to leaf orientation, and therefore on  
 258 APAR<sub>green</sub> and the local leaf physiology (*e.g.*, leaf sun and shade adaptations). SIF emission  
 259 yield informs us on the 2<sup>nd</sup> process. It is defined as:

$$\text{SIF emission yield} = \frac{\text{SIF}_{\text{emitted}}}{\text{APAR}_{\text{green}}}. \quad (1)$$

260 Since satellite and airborne spectrometers only measure SIF radiation that exits a canopy, the  
 261 3<sup>rd</sup> process is investigated through the so-called SIF escape factor<sub>hemi</sub>:

$$\text{SIF escape factor}_{\text{hemi}} = \frac{\text{SIF}_{\text{exitance}}}{\text{SIF}_{\text{emitted}}} \quad (2)$$

262 where  $SIF_{\text{exitance}}$  is the total SIF radiation exiting the top of the canopy in all directions of the  
 263 upper hemisphere. SIF escape factor  $_{\text{hemi}}$  was computed for the chlorophyll fluorescence  
 264 peaks located at 640 – 700 nm and 700 – 850 nm spectral regions.

265 SIF sensors generally measure from a unique viewing direction. Hence, the directional SIF  
 266 nadir escape factor was also studied:

$$\text{SIF escape factor}_{\text{nadir}} = \frac{\pi \cdot SIF_{\text{nadir radiance}}}{SIF_{\text{emitted}}} \quad (3)$$

267 SIF escape factor  $_{\text{nadir}}$  was also computed for the chlorophyll fluorescence peaks located at  
 268 640 – 700 nm and 700 – 850 nm spectral regions.

269 Finally, the combination of the 2<sup>nd</sup> and the 3<sup>rd</sup> processes was in the case of a nadir observation  
 270 evaluated with the SIF nadir yield ( $\text{sr}^{-1}$ ) (van der Tol et al., 2019):

$$\text{SIF nadir yield} = \frac{SIF_{\text{nadir radiance}}}{APAR_{\text{green}}} \quad (4)$$

271 where  $SIF_{\text{nadir radiance}}$  is a SIF flux ( $\text{W} \cdot \text{m}^{-2} \cdot \text{sr}^{-1}$ ), that is for example recorded by an optical  
 272 remote sensing sensor in the nadir viewing direction.

273

## 274 2.7. Canopy structure error assessment

275 The impact of forest architecture on diurnal SIF emission and nadir observation was assessed  
 276 as the relative errors made on SIF quantities that are simulated with mock-ups (*i.e.*, 1D, 0D)  
 277 with simplified architecture, taking the quantities simulated with the 3D mock-ups as reference.

278 The influence of forest 3D structure on SIF observation was assessed by comparing the DART-  
 279 Lux top-of-canopy (TOC) nadir SIF radiance  $L_v$  (PSI, PSII and total), of the 3D, 1D and 0D  
 280 mock-ups of the eight forest sites simulated. Two types of relative errors were computed:

281 - Per spectral band for a specific time (*e.g.*, 12.00 local time), by computing the relative errors

282  $\epsilon_{SIF, L_v, iD-3D}(\lambda)$  where  $i \in \{0, 1\}$ :

$$\epsilon_{SIF, L_v, iD-3D}(\lambda) = 100\% \times \frac{SIF_{\text{radiance}, iD}(\lambda) - SIF_{\text{radiance}, 3D}(\lambda)}{SIF_{\text{radiance}, 3D}(\lambda)} \quad (5)$$

283

284 - Per hour from 7.00 to 19.00, by computing mean absolute relative errors (MARE) for the  
 285 two 640 – 700 nm and 700 – 850 nm spectral regions:

$$MARE_{SIF,Lv,1D-3D}(t) = \frac{1}{\sum_i \Delta\lambda_i} \cdot \sum_i \frac{|SIF_{radiance,1D}(t, \lambda) - SIF_{radiance,3D}(t, \lambda)|}{SIF_{radiance,3D}(t, \lambda)} \cdot \Delta\lambda_i \quad (6)$$

286

287 Using 3D plots as reference, the influence of canopy architecture was also assessed for:

288 - Nadir reflectance  $\rho$ : relative errors  $\varepsilon_{\rho,0D-3D}(\lambda)$  and  $\varepsilon_{\rho,1D-3D}(\lambda)$  of 0D and 1D plots, as well as  
 289  $MARE_{\rho,1D-3D}(t)$  of 1D plots.

290 - APAR<sub>green</sub>: relative error  $\varepsilon_{APAR,1D-3D}(t)$  of 1D plots.

291 - SIF emission yield: relative error  $\varepsilon_{SIF.EY,1D-3D}(t)$  of 1D plots.

292 - SIF<sub>emitted</sub>: relative error  $\varepsilon_{SIF.em,1D-3D}(t)$  of 1D plots.

293 -SIF escape factor<sub>hemi</sub> and SIF escape factor<sub>nadir</sub>: relative errors  $\varepsilon_{SIF.EF,1D-3D}(t)$  of 1D plots  
 294 at 640 – 700 nm and 700 – 850 nm spectral regions.

295 - SIF nadir yield: relative errors  $\varepsilon_{SIF.NY,1D-3D}(t)$  of 1D plots at 640 - 700 nm and 700 - 850 nm.

296 with relative error for a given quantity  $Q$  equal to  $\varepsilon_{Q,1D-3D}(t) = 100\% \times \frac{Q_{1D}(t) - Q_{3D}(t)}{Q_{3D}(t)}$ .

## 297 **2.8. Influence of canopy wood on SIF emission and measurements**

298 Although they do not intrinsically emit fluorescence, woody elements impact the RB and SIF  
 299 observations through their interaction with PAR and SIF. They give rise to two major effects.

300 i) Shading effect: woody elements shade foliar elements, which lowers leaf irradiance and  
 301 subsequently SIF emission. ii) Blocking effect: woody elements intercept the emitted SIF  
 302 radiation, preventing it from escaping the canopy. These two effects are not independent, due  
 303 to sky radiation and multiple scattering and re-absorption mechanisms in the canopy. For  
 304 example, the same woody element can shade a leaf element and block its SIF radiation.

305

306 DART simulations were used to quantify the influence of woody elements on SIF observation,  
 307 and to separate the shading and blocking effects of woody elements for the CM1 and LM2 sites.

308 For that, theoretical “no wood” (NW) scenes were constructed by removing cells corresponding  
 309 to woody elements from the original “with wood” 3D mock-ups (W). It allowed us to compare

310 the DART-Lux top-of-canopy (TOC) nadir SIF radiance (PSI, PSII and total) of the (W) and  
 311 (NW) abstractions, and to compute two types of relative error:

312 - Per spectral band for a specific time (*e.g.*, 12.00 local time):

$$\varepsilon_{SIF,Lv,NW-W}(\lambda) = 100\% \times \frac{SIF_{radiance,NW}(\lambda) - SIF_{radiance,W}(\lambda)}{SIF_{radiance,W}(\lambda)} \quad (7)$$

313 - Per hour from 7.00 to 19.00, by computing mean absolute relative errors for the 640 – 700  
 314 nm and 700 – 850 nm spectral regions:

$$MARE_{SIF,Lv,NW-W}(t) = \frac{1}{\sum_i \Delta\lambda_i} \cdot \sum_i \frac{|SIF_{radiance,NW}(t, \lambda) - SIF_{radiance,W}(t, \lambda)|}{SIF_{radiance,W}(t, \lambda)} \cdot \Delta\lambda_i \quad (8)$$

315 Using W plots as reference, the influence of woody elements was assessed for:

316 - APAR<sub>green</sub> (shading effect): relative error  $\varepsilon_{APAR,NW-W}(t)$  NW.

317 - SIF nadir escape factor SIF<sub>nadir EF</sub> (blocking effect): relative error  $\varepsilon_{SIF,NEF,NW-W}(t)$  of NW  
 318 plots, where:

$$SIF_{nadir EF} = \frac{\pi \cdot SIF_{nadir radiance}}{SIF_{emitted}} \quad (9)$$

319 With the relative error for a given quantity  $Q$  equal to:

$$\varepsilon_{Q,NW-W}(t) = 100\% \times \frac{Q_{NW}(t) - Q_W(t)}{Q_W(t)} \quad (10)$$

320

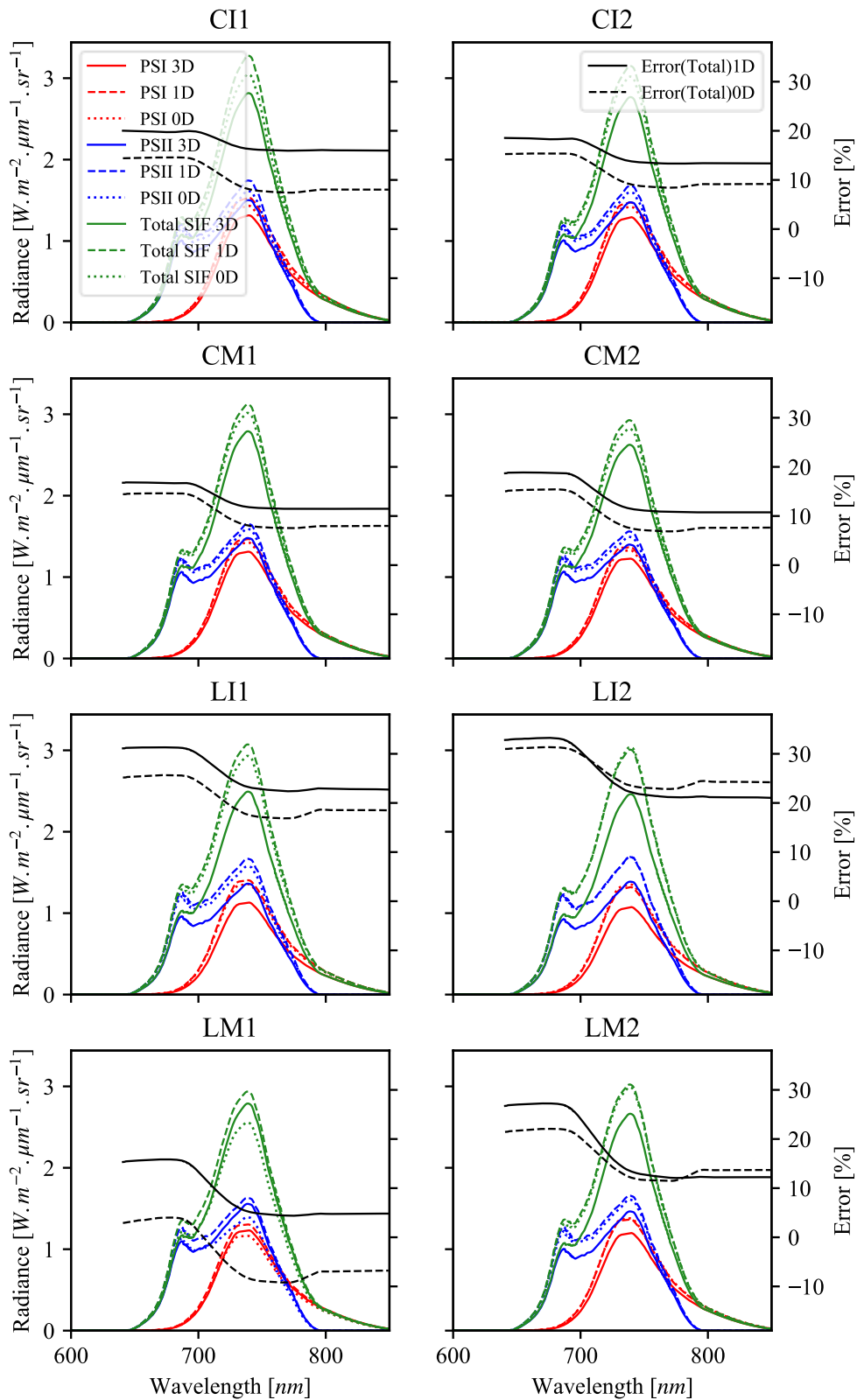
### 321 **3. Results**

#### 322 **3.1. General influence of forest abstractions on SIF nadir observations**

323 Figure 4 shows the PSI, PSII and total SIF nadir radiance of the 8 forest plots simulated with  
 324 3D, 1D and 0D mock-ups at 12.00 (SZA = 21.050°, SAA = 47.256°).  $\varepsilon_{SIF,Lv,0D-3D}(\lambda)$  and  
 325  $\varepsilon_{SIF,Lv,1D-3D}(\lambda)$  quantify the relative errors associated with the 0D and 1D forest plots. For all  
 326 plots, the 1D mock-ups give the largest nadir total SIF, PSI and PSII radiance.  $\varepsilon_{SIF,Lv,1D-3D}$   
 327 illustrates the influence of the forest horizontal heterogeneity on radiation propagation in forest,  
 328 since the canopy horizontal heterogeneity is the only difference between 3D and 1D mock-ups.  
 329 These larger values of 1D SIF radiance can be explained by the fact that the top layers of 1D

330 plots intercept more radiation than the top layers of 3D plots (i.e., clumping effect), which gives  
331 rise to larger SIF emission by canopy layers that tend to contribute most to the canopy SIF  
332 radiance. Also, the ground is more visible in 3D plots than 1D plots, whereas the ground has no  
333 SIF emission. The order of magnitude of the difference between the radiance of 1D and 3D  
334 mockups is similar for all investigated forest sites.





335

336

337

338

Figure 4. PSI, PSII and total SIF nadir radiance of the eight sites simulated with 3D, 1D and 0D abstractions, at 12.00 local time ( $SAZ = 21.050^\circ$ ,  $SAA = 47.256^\circ$ ).

339 SIF radiance values of 0D and 1D forest mock-ups differ due to differences in the leaf and wood  
 340 vertical distributions, which vary greatly among the sites (except for LI2 and LM2). In general,  
 341 nadir SIF radiance relative differences  $\varepsilon_{SIF,L_v,0D-1D}(\lambda)$  between 0D and 1D plots are much  
 342 smaller than  $\varepsilon_{SIF,L_v,1D-3D}(\lambda)$  between 1D and 3D plots, except for LM1. It means that forest  
 343 horizontal heterogeneity has a larger influence on SIF radiance than forest vertical  
 344 heterogeneity. SIF radiance was always smaller for 0D mock-ups than for 1D mockups. This is  
 345 mostly explained by the homogenized vertical distribution of both foliar and woody elements  
 346 in the 0D abstractions compared to 1D abstractions. For example, in CI1, CI2, CM1 and CM2,  
 347 leaf density is higher in upper canopy layers (Figure 14), foliar homogenization increases the  
 348 density of foliar elements in the canopy bottom layers, which increases the canopy shading and  
 349 blocking effects. For LI2, the situation is different because leaf density is highest in the lower  
 350 canopy layers. Therefore, foliar homogenization increases leaf density in the canopy upper  
 351 layers, which decreases the canopy shading and blocking effects. These trends are also  
 352 influenced by the vertical distribution of woody elements.

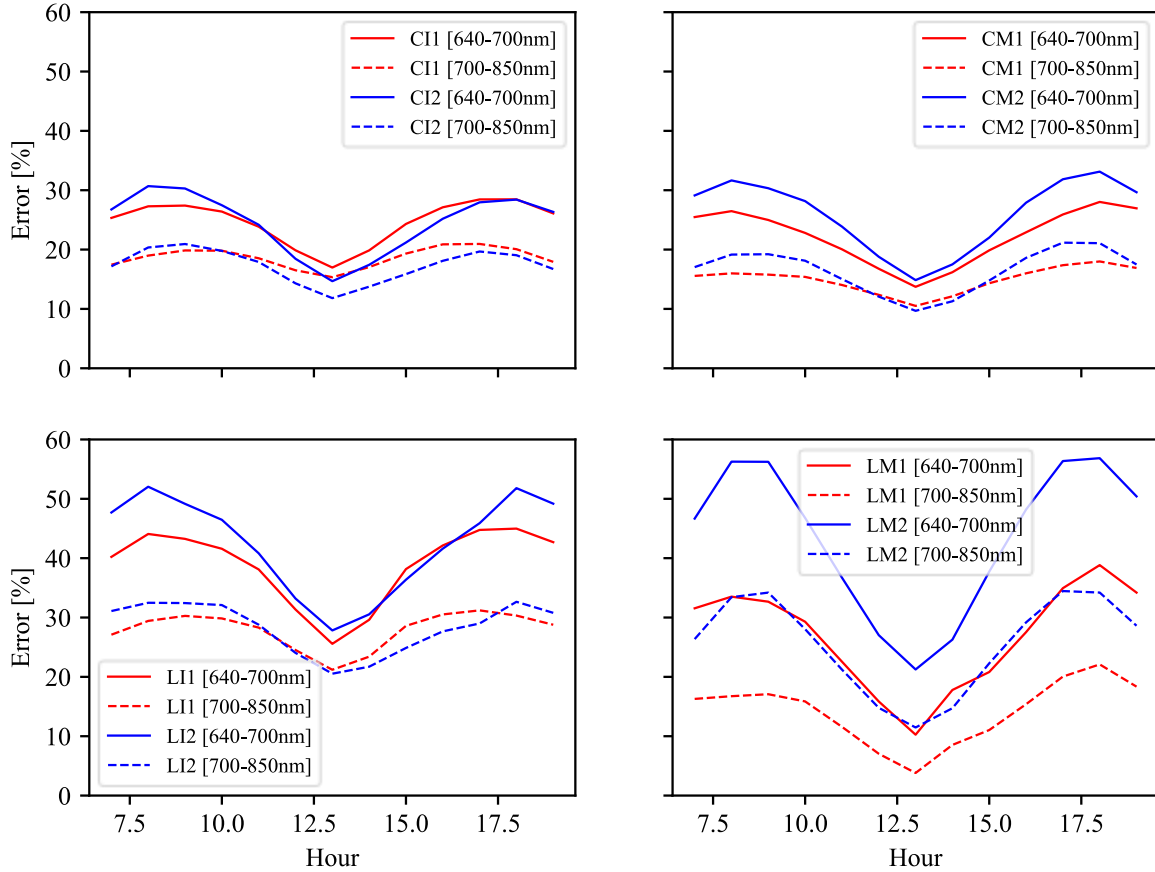
353 The relative difference  $\varepsilon_{SIF,L_v,0D-3D}(\lambda)$  between the radiance of 0D and 3D mock-ups is driven  
 354 by horizontal and vertical heterogeneity. The inequality  $\varepsilon_{SIF,L_v,0D-3D}(\lambda) < \varepsilon_{SIF,L_v,1D-3D}(\lambda)$   
 355 indicates that vertical and horizontal heterogeneities have an opposite effect on canopy SIF  
 356 radiance in our simulations. While the horizontal heterogeneity tends to decrease canopy SIF  
 357 nadir radiance, the vertical heterogeneity tends to increase it. LM1 is an exception. Its 0D SIF  
 358 radiance is lower than its 3D SIF radiance in the NIR domain. It means that its vertical  
 359 heterogeneity imposes a larger influence on SIF nadir radiance than its horizontal heterogeneity,  
 360 which is consistent with the fact that LM1 is the only plot where the density of woody and foliar  
 361 elements is very dense in the lower canopy layers.

362

363 Figure 5 shows the diurnal evolution of  $MARE_{SIF,L_v,1D-3D}(t)$  (*i.e.*, relative error of total nadir  
 364 SIF radiance of 1D plots compared to 3D plots) at 640 - 700 nm and 700 - 850 nm. This quantity  
 365 is mostly influenced by the forest horizontal heterogeneity. It appears symmetrically distributed  
 366 between the morning and the afternoon hours, with a dip appearing always at local noon. It is  
 367 the largest around 8.00 and 18.00, reaching up to 55%, and the smallest at 13.00 (local solar  
 368 noon), with values between 10% and 20%. It is usually larger at 640 - 700 nm than at 700 - 850  
 369 nm, where shading effects are dampened by prevailing multiple scattering events. This diurnal  
 370 variation can be explained by the shadow effects associated with changing solar zenith angle

371 and associated variability in the proportions of direct sun and diffuse atmospheric radiation. In  
 372 the early morning, it starts increasing because shadow effects are increasing due to the increase  
 373 of the direct sun proportion in total irradiance. Later in the morning, it starts decreasing because  
 374 shadow effects decrease due to the decrease of solar zenith angle, reaching a minimum at solar  
 375 noon. A symmetrical behavior starts in the second half of the day.

376



377

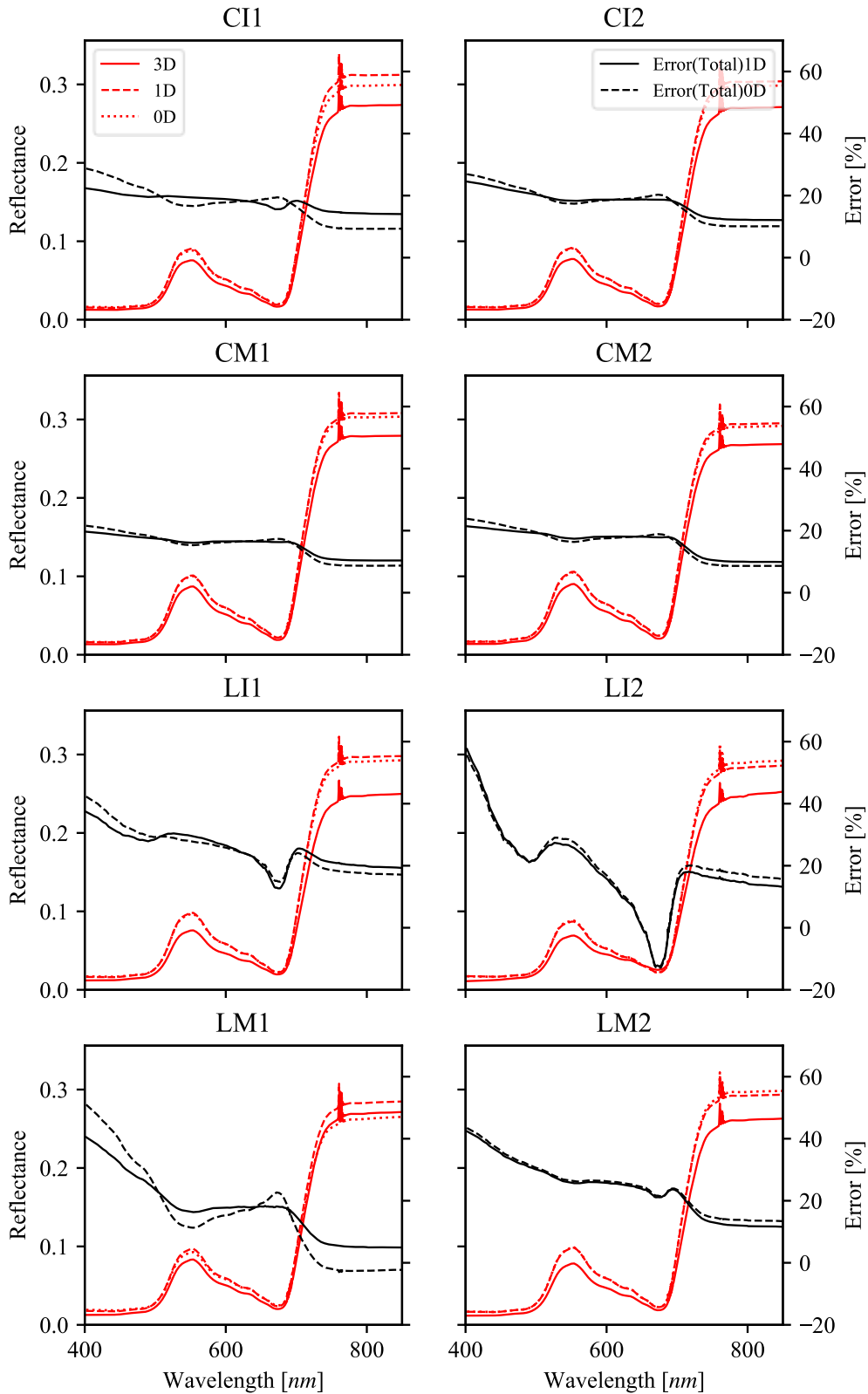
378 Figure 5. Diurnal evolution of the total nadir SIF radiance relative error  $MARE_{SIF,L,1D-3D}(t)$   
 379 between 1D and 3D mock-ups at 640 – 700 nm and 700 – 850 nm.

380 Figure 6 shows the canopy nadir reflectance of the 8 forest plots simulated with 3D, 1D and 0D  
 381 mock-ups at 12.00 (SZA = 21.050°, SAA = 47.256°).  $\epsilon_{\rho,0D-3D}(\lambda)$  and  $\epsilon_{\rho,1D-3D}(\lambda)$  quantify  
 382 the of 0D and 1D abstractions compared to 3D abstraction. All curves have the expected local  
 383 spectral peak around the O<sub>2</sub>-A absorption band at 760nm. As for the SIF radiance (Figure 4),  
 384 the total reflectance of 3D plots is the smallest compared to the 1D and 0D plots, except for  
 385 LM1 where the 0D plot has a slightly lower reflectance than the 3D plot above 700nm.

386 Therefore, as for SIF radiance, the horizontal heterogeneity tends to decrease the nadir  
387 reflectance.

388 The influence of the vertical heterogeneity of the plots on their reflectance is not as clear as for  
389 SIF radiance. By contrast to the relative errors on the SIF radiance, the relative errors on the  
390 total reflectance of the 1D and 0D forest plots are similar. This stresses two points. 1) As for  
391 SIF, the forest vertical heterogeneity plays a lesser role than the forest horizontal heterogeneity.  
392 2) The vertical heterogeneity plays a larger role for canopy SIF radiance than for canopy  
393 radiance that contains radiance due to the scattering of solar radiation. Also, these relative errors  
394 tend to higher for wavelengths under 700nm. Indeed, the 1D and 0D abstractions of the forest  
395 cover neglect the shadow effects due to direct and diffuse radiation and canopy structure.  
396 Multiple scattering being smaller at wavelengths lower than 700nm, shadowing effects are  
397 larger in these wavelengths. The diurnal evolutions of the relative error  $MARE_{\rho,1D-3D}(t)$  in  
398 nadir reflectance of 1D plots at 640-700 nm and 700-850 nm (Figure 7) have shapes and orders  
399 of magnitude similar to those of SIF radiance  $MARE_{SIF,L,1D-3D}$  (Figure 5), except for LI2 at  
400 640 - 700nm, where the relative error is higher for SIF radiance.

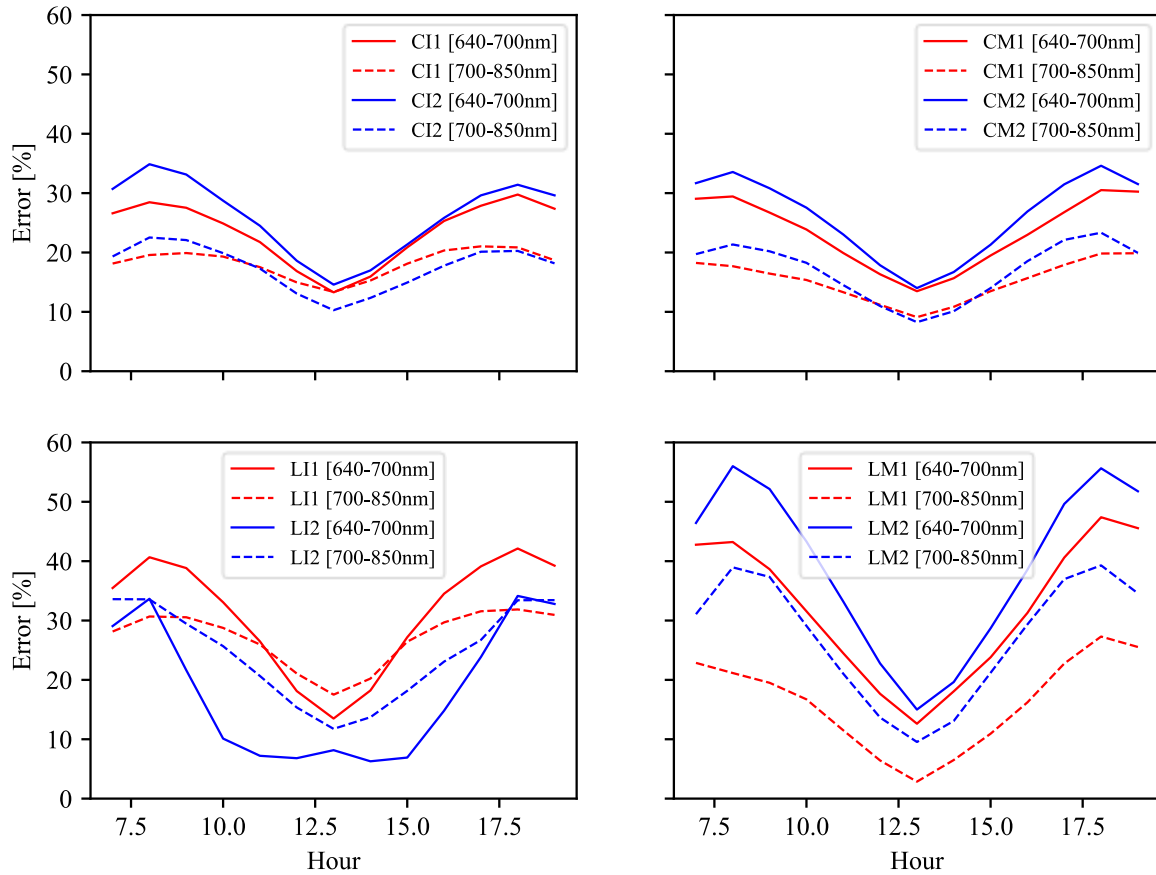
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402  
403  
404  
405

Figure 6: Canopy nadir reflectance of the eight study sites simulated with 3D, 1D and 0D mock-ups, at 12.00 local time (SZA = 21.050°, SAA = 47.256°).  $\epsilon_{\rho,1D-3D}(\lambda)$

406

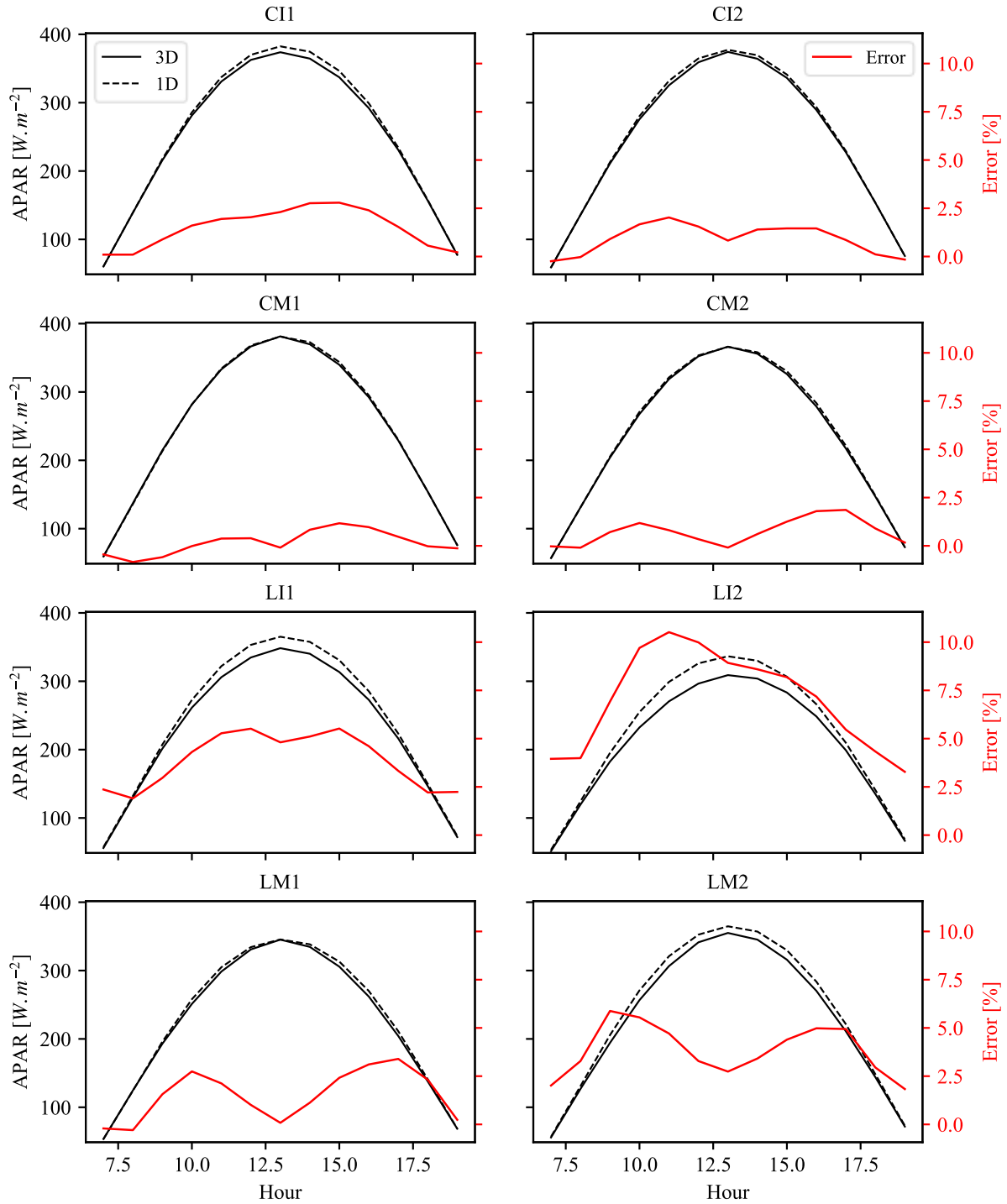


407

408 Figure 7: Diurnal evolution of canopy nadir reflectance relative error  $MARE_{\rho,1D-3D}$  at 640-700 nm  
 409 and 700-850 nm due to differences in horizontal heterogeneity in 1D and 3D mock-ups.  
 410

### 411 3.2. Impact of forest 3D structure on $APAR_{green}$ (1<sup>st</sup> process)

412 Figure 8 shows the diurnal PAR absorbed by green leaves ( $APAR_{green}$ ) in the eight 3D and 1D  
 413 forest mock-ups, and their associated relative error  $\varepsilon_{APAR,1D-3D}(t)$ . The 3D mock-ups have  
 414 smaller  $APAR_{green}$  than the 1D mock-ups. This is consistent with the larger reflectance of 1D  
 415 mock-ups compared to the 3D mock-ups, due to the horizontal heterogeneity of the forest plots.  
 416  $\varepsilon_{APAR,1D-3D}(t)$  is usually smaller than 5%, with a maximum of 10% for LI2 before noon. It is  
 417 smaller than the relative difference of nadir SIF radiance between 3D and 1D forest abstractions  
 418 (Figure 5). This indicates that even though the  $APAR_{green}$  diurnal changes play an important  
 419 role, they are not the only cause responsible for the relative difference in the nadir SIF radiance.  
 420



421

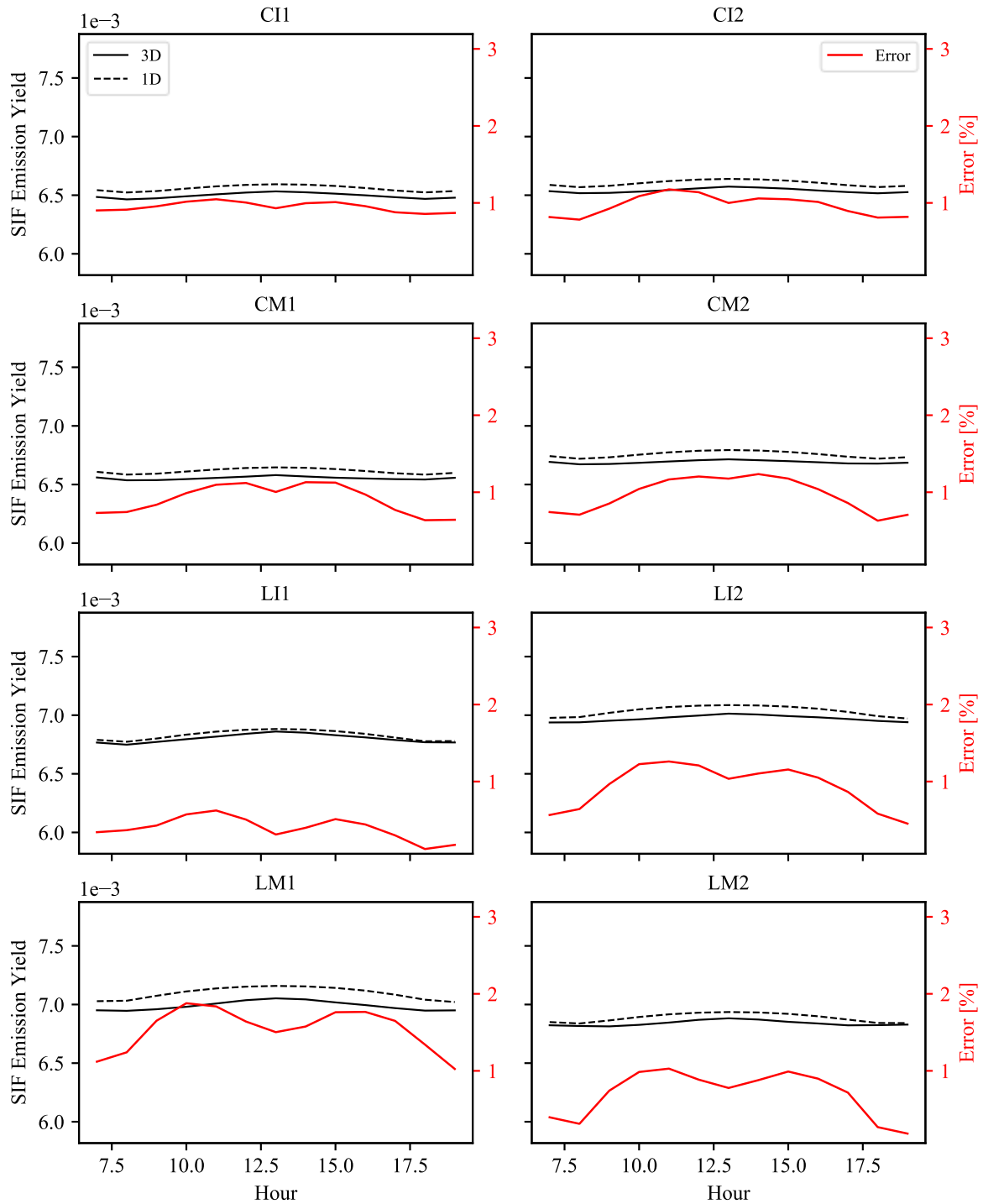
422 Figure 8. Diurnal PAR absorbed by green leaves ( $APAR_{green}$ ) in 3D and 1D forest abstractions of the  
 423 eight study sites, and their associated relative error  $\varepsilon_{APAR,1D-3D}(t)$  triggered by changes in  
 424 horizontal heterogeneity of the forest abstractions.  
 425

426

### 3.3. Impact of forest 3D structure on leaf SIF emission yield (2<sup>nd</sup> process)

427 Figure 9 shows the diurnal total SIF emission yield for 3D and 1D mock-ups and the associated  
428 diurnal relative error  $\varepsilon_{SIF.EY,1D-3D}(t)$  due to horizontal heterogeneity differences. Relative  
429 errors are similar and small for all plots. They reveal that in our simulations the impact of forest  
430 3D architecture on SIF emission yield in our simulations is of a less importance. The almost  
431 constant diurnal response due to our modeling assumption of constant leaf SIF properties  
432 throughout the day.  
433





434

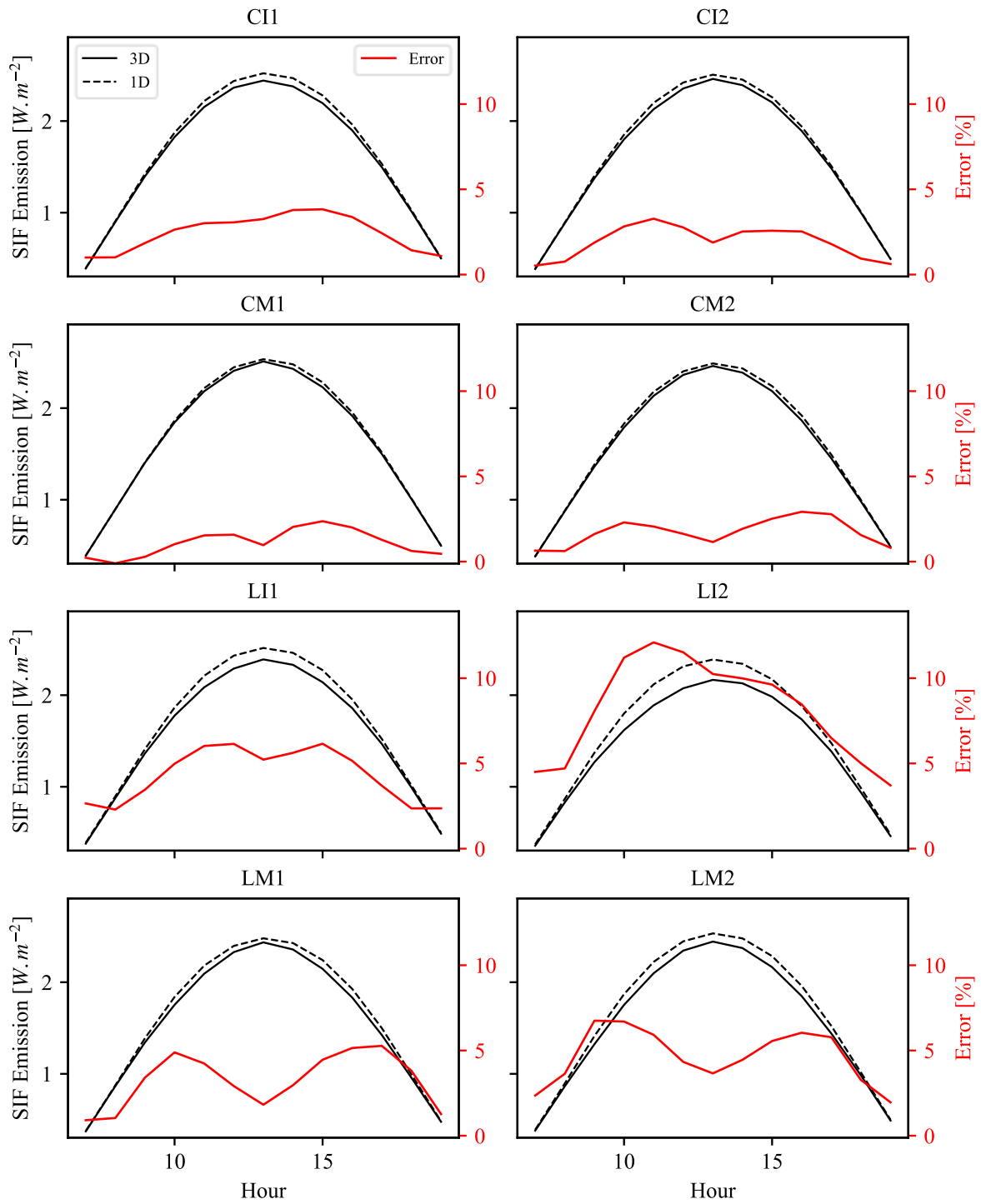
435 Figure 9. Diurnal SIF emission yield of the 3D and 1D forest mock-ups and relative  
 436 errors  $\varepsilon_{SIF.EY,1D-3D}(t)$   
 437

438 Since SIF emission yield in our simulations is hardly affected by the forest 3D architecture, the  
 439 diurnal behavior of the DART-FT simulated leaf SIF emission (Figure 10) is understandably  
 440 very similar to that of  $APAR_{green}$  (Figure 8). The relative error  $\varepsilon_{SIF.em,1D-3D}(t)$  computed

441 between the 3D and 1D forest abstractions (Figure 10) gathers the combined errors related to  
442 both the 1<sup>st</sup> and the 2<sup>nd</sup> processes, without being a simple addition of their relative errors.

443 Figure 11 plots the vertical profiles of LAI, and SIF emission in 3D and 1D plots. The LAI of  
444 a layer  $i$  located between  $[i m, (i + 1) m]$  is the total foliar area of this layer divided by the  
445 scene area. It shows that the overestimation of the SIF emission in 1D plots compared to 3D  
446 plots mainly occurs in the canopy top layers, *i.e.*,  $SIF_{\text{emitted},1D} > SIF_{\text{emitted},3D}$  in these layers.  
447 Also, SIF emission is underestimated in the lower layers of 1D plots. Indeed, in 3D forest mock-  
448 ups, the forest horizontal heterogeneity leads to better illumination of the lower layers.

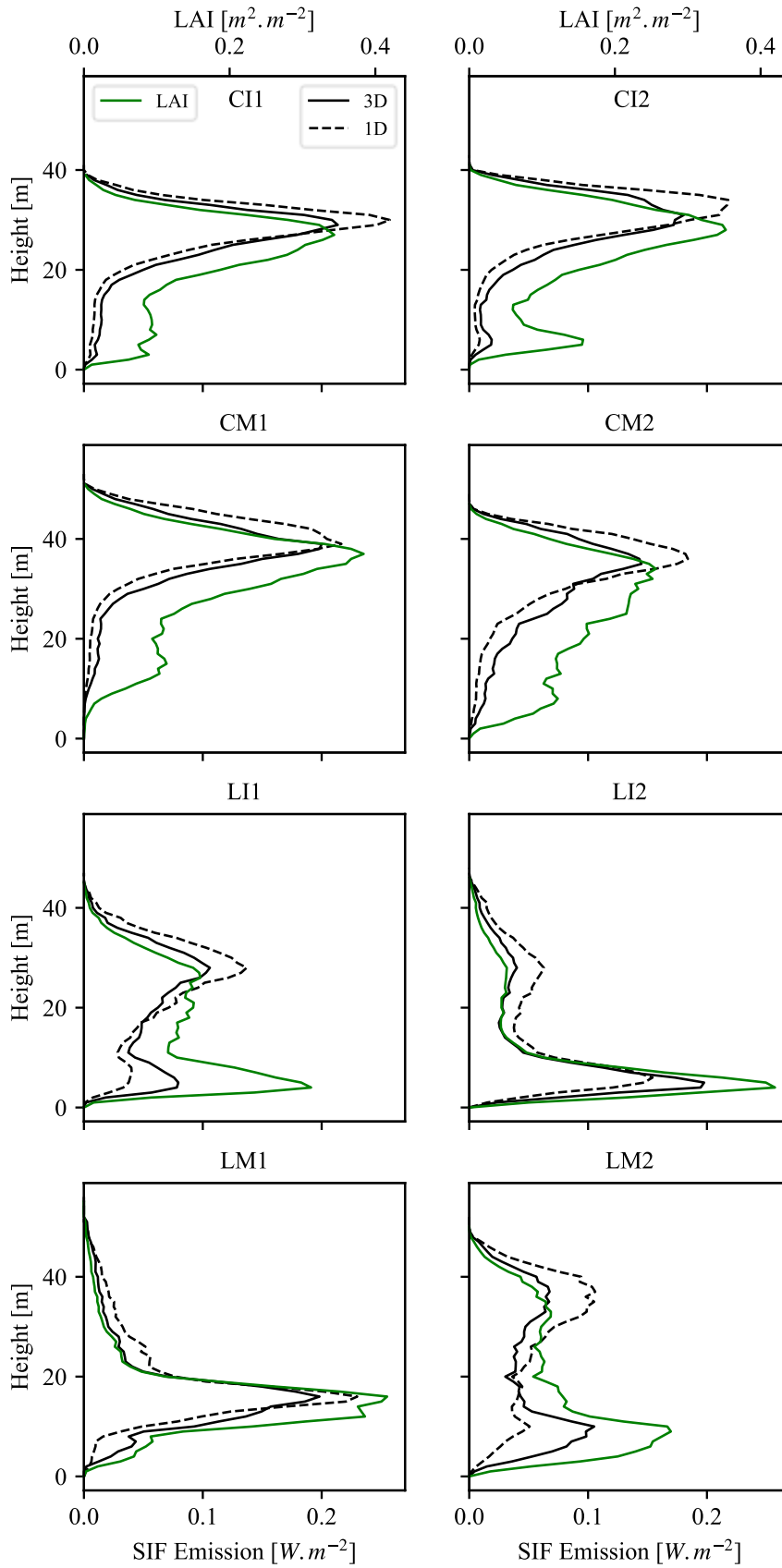
449



450

451 Figure 10. Diurnal leaf SIF emissions for the 3D and 1D forest abstractions and their associated relative  
 452 errors  $\varepsilon_{SIF.em,1D-3D}(t)$ .  
 453

454



455

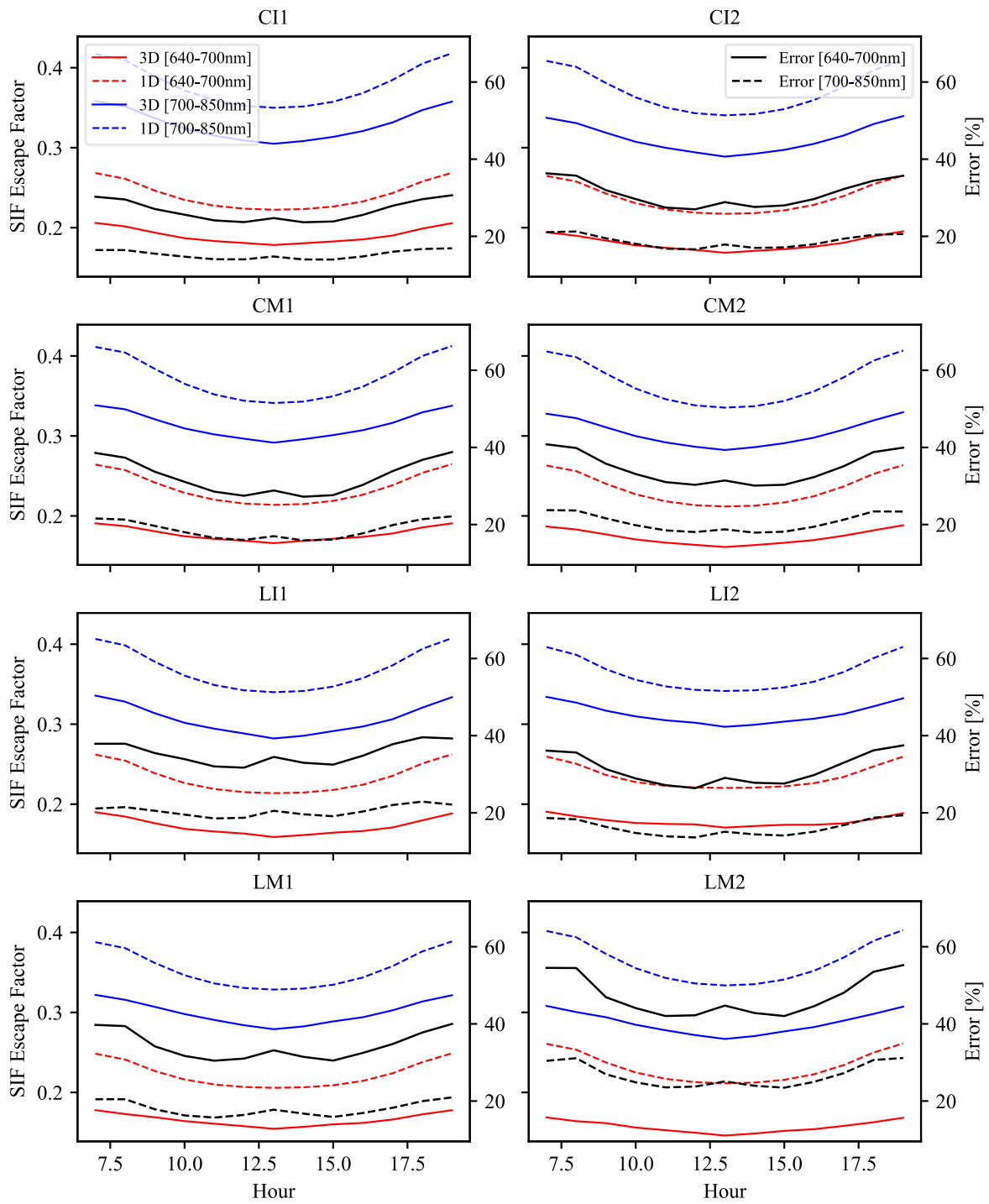
456

Figure 11. Vertical profiles of LAI and leaf SIF emission at 12.00 (local time).

457 **3.4. Impact of forest 3D structure on SIF escape factor (3<sup>rd</sup> process)**

458 Figure 12 and Figure 13 show the diurnal SIF escape factor<sub>hemi</sub> and SIF escape factor<sub>nadir</sub> of 3D  
459 and 1D plots at 640 - 700 nm and 700 nm - 850 nm, and their relative errors  $\varepsilon_{SIF.EF,1D-3D}(t)$   
460 and  $\varepsilon_{SIF.EFnadir,1D-3D}(t)$  are larger (*e.g.*, > 50% for LM2) than for APAR<sub>green</sub> (Figure 8) and  
461 leaf SIF emission (Figure 10). Therefore, the 3<sup>rd</sup> process is more affected by forest 3D structure  
462 than the first two processes. The SIF escape factor is systematically overestimated in 1D plots.  
463 It is larger at 700 nm - 850 nm than at 640 - 700 nm, due to more important multiple scattering  
464 mechanisms, which results in lower relative errors at 700 nm - 850 nm than at 640 - 700 nm.

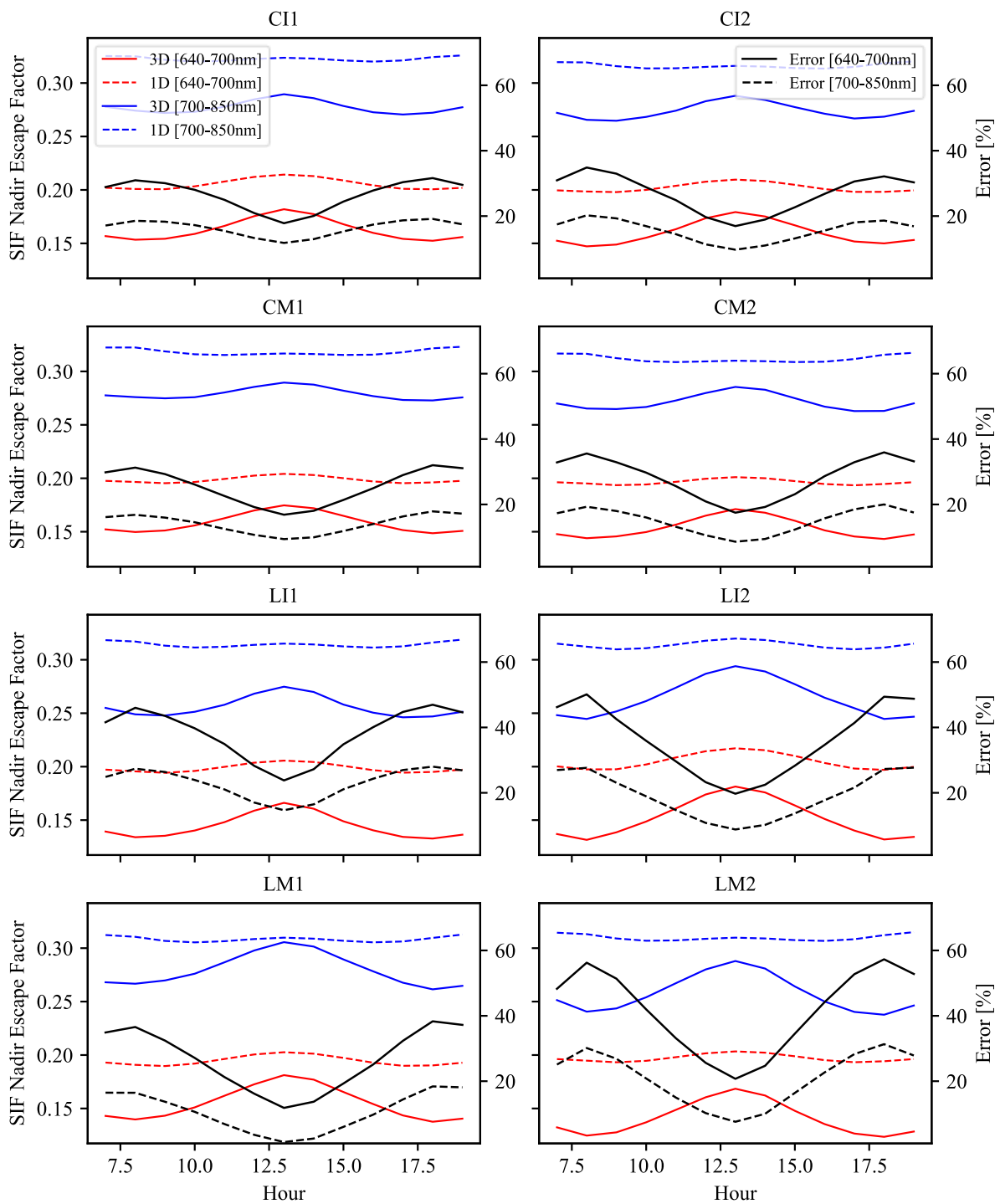
465 The SIF photons that cannot escape the canopy are absorbed by the canopy elements (*i.e.*, leaves,  
466 woody elements, ground). The overestimation of the SIF escape factor of 1D plots compared  
467 to 3D plots is also reflected by a higher absorption of SIF photons in 3D plots (Table 6, Table  
468 7). We can note that the ground absorption is greatly underestimated in 1D forest abstractions.  
469 Again, this is explained by the forest horizontal heterogeneity.



470

471 Figure 12. Diurnal SIF escape factor<sub>hemi</sub> of the 3D and 1D plots and their associated relative errors.

472



473

474 Figure 13: Diurnal SIF escape factor<sub>nadir</sub> of the 3D and 1D plots and their associated relative errors.

475

476 Figure 14 shows the vertical profiles of LAI, woody elements (defined similarly as the vertical  
 477 profile of LAI), and SIF absorption in 3D and 1D plots. The vertical profiles of SIF absorption

478 show that in 1D forest abstractions, absorption is overestimated in the top layers and  
 479 underestimated in the bottom layers as for the leaf SIF emission profiles (Figure 11).

480

481 Table 6. SIF absorption by the ground and vegetation (leaves and wood) (640-700nm) at 12pm

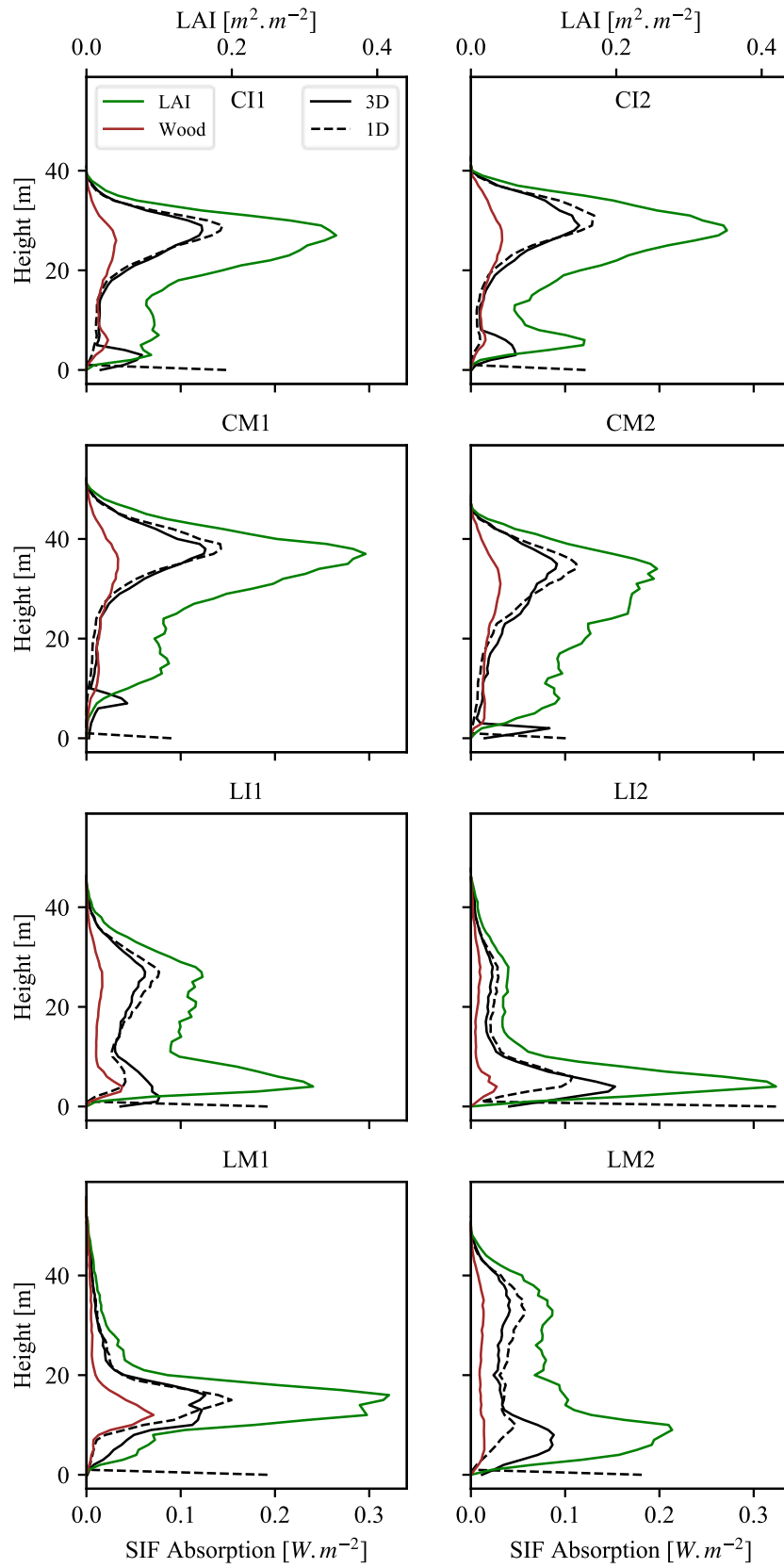
Plot	CI1	CI2	CM1	CM2	LI1	LI2	LM1	LM2
Fraction of emitted SIF absorbed by "Ground" (3D)	0,0310	0,0290	0,0230	0,0272	0,0463	0,0704	0,0486	0,0449
Fraction of emitted SIF absorbed by "Ground" (1D)	0,0216	0,0180	0,0130	0,0160	0,0301	0,0584	0,0329	0,0274
Relative difference (%)	-30,28	-38,19	-43,40	-41,38	-35,14	-17,12	-32,44	-38,97
Fraction of emitted SIF absorbed by "Leaves + Wood" (3D)	0,7765	0,7838	0,7903	0,7912	0,7757	0,7352	0,7636	0,7843
Fraction of emitted SIF absorbed by "Leaves + Wood" (1D)	0,7512	0,7545	0,7616	0,7613	0,7461	0,7073	0,7462	0,7492
Relative difference (%)	-3,26	-3,74	-3,63	-3,78	-3,81	-3,79	-2,28	-4,47
Absorption fraction (3D)	0,8075	0,8129	0,8133	0,8184	0,8220	0,8056	0,8123	0,8291
Absorption fraction (1D)	0,7728	0,7725	0,7746	0,7772	0,7762	0,7657	0,7791	0,7766
Relative difference (%)	-4,30	-4,97	-4,76	-5,03	-5,57	-4,95	-4,09	-6,34

482

483 Table 7. SIF absorption by the ground and vegetation (leaves and wood) (700-850nm) at 12pm.

Plot	CI1	CI2	CM1	CM2	LI1	LI2	LM1	LM2
Fraction of emitted SIF absorbed by "Ground" (3D)	0,0905	0,0842	0,0683	0,0768	0,1249	0,1741	0,1282	0,1249
Fraction of emitted SIF absorbed by "Ground" (1D)	0,0716	0,0593	0,0440	0,0502	0,0941	0,1640	0,0952	0,0887
Relative difference (%)	-20,96	-29,52	-35,50	-34,62	-24,68	-5,78	-25,71	-28,95
Fraction of emitted SIF absorbed by "Leaves + Wood" (3D)	0,6194	0,6369	0,6543	0,6600	0,6062	0,5265	0,5897	0,6185
Fraction of emitted SIF absorbed by "Leaves + Wood" (1D)	0,6133	0,6257	0,6453	0,6482	0,5991	0,5098	0,6037	0,6057
Relative difference (%)	-0,98	-1,77	-1,39	-1,79	-1,16	-3,19	2,38	-2,08
Absorption fraction (3D)	0,7099	0,7211	0,7226	0,7369	0,7311	0,7006	0,7179	0,7434
Absorption fraction (1D)	0,6849	0,6850	0,6893	0,6985	0,6932	0,6738	0,6989	0,6944
Relative difference (%)	-3,53	-5,01	-4,61	-5,21	-5,18	-3,83	-2,64	-6,59





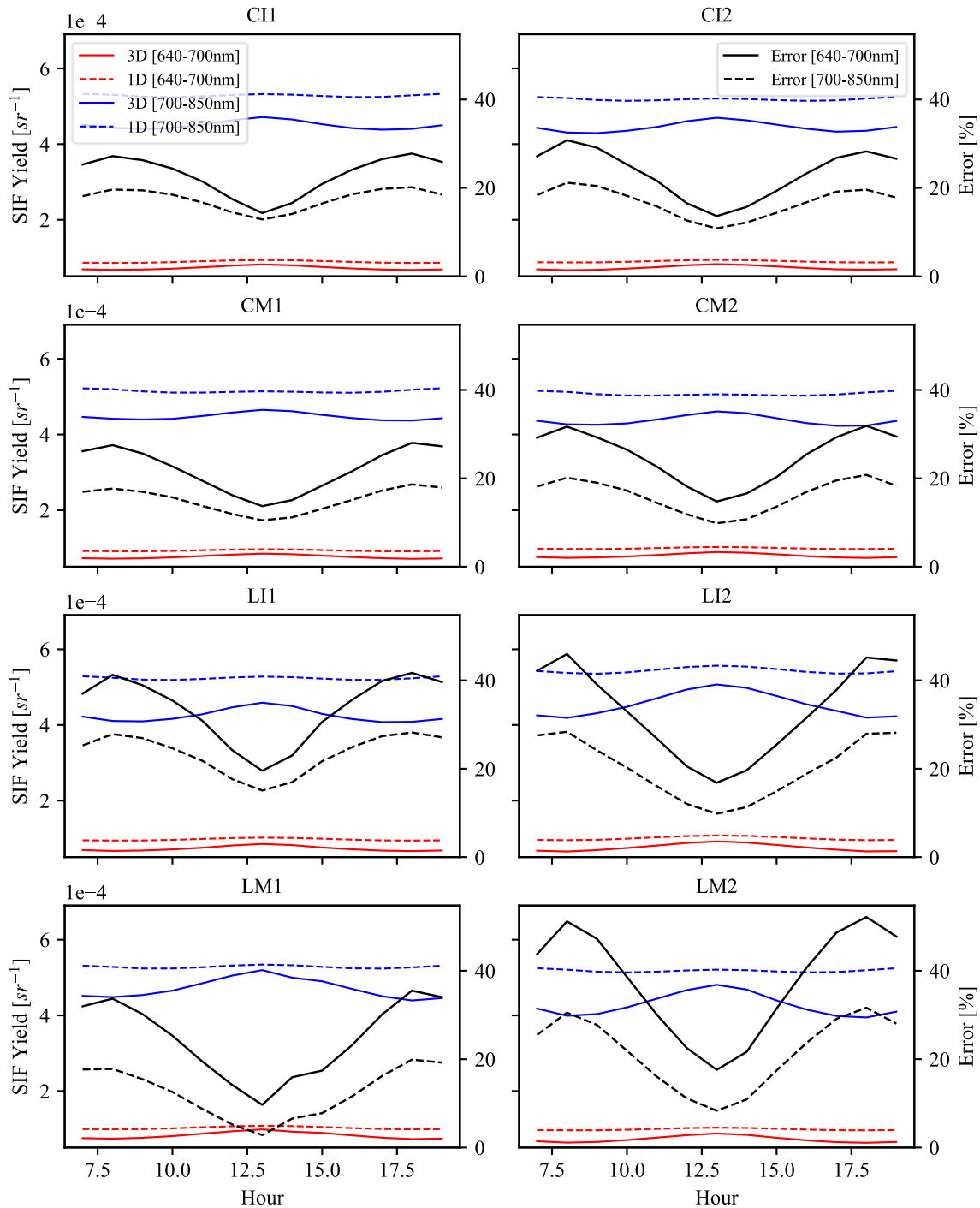
484

485 Figure 14. Vertical profiles of LAI, woody elements and SIF absorption in 3D and 1D forest  
 486 abstractions, at 12.00 (local time).

487  
488  
489

### 3.5. Impact of forest 3D structure on SIF nadir yield (2<sup>nd</sup> and 3<sup>rd</sup> processes)

490 Figure 15 shows diurnal values of SIF nadir yield for 3D and 1D forest plots and their relative  
491 error  $\varepsilon_{SIF.NY,1D-3D}(t)$ . SIF nadir yield informs on the potential of nadir viewing remote sensing  
492 instruments to observe leaf SIF emission. The diurnal evolution of  $\varepsilon_{SIF.NY,1D-3D}$  is similar to  
493 the diurnal evolution of total nadir SIF radiance relative error  $MARE_{SIF,L_v,1D-3D}$  (Figure 5):  
494 larger errors occur in early morning around 8:00 and late afternoon around 18:00, with minimal  
495 errors at noon. SIF yield of 1D plots is always overestimated. Also, errors are larger at 640 nm  
496 - 700 nm than at 700 - 850 nm. This is due to the lower impact of multiple scattering at 640 -  
497 700 nm than at 700 - 850 nm and therefore the larger impact of shadowing effects at 640 - 700  
498 nm.



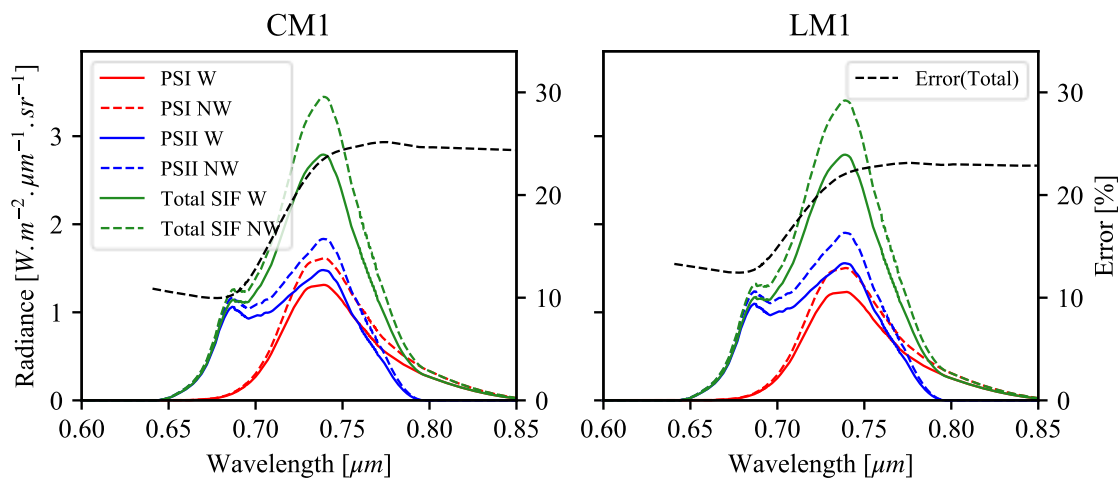
499  
 500 Figure 15. Diurnal SIF nadir yield of 3D and 1D plots and relative errors at 640 - 700 nm and 700 - 850 nm.

501 **3.6. Influence of woody elements**

502 Figure 16 illustrates the impact of woody elements (*i.e.*, branches and trunks) on the canopy  
 503 SIF signal. It shows PSI, PSII and total SIF nadir spectral radiance at 12.00 of local time for  
 504 CM1 and LM1 3D plots simulated with (W) and without (NW) woody elements, and also the

505 associated relative errors  $\varepsilon_{SIF,L,NW-W}(\lambda)$  for the total SIF nadir radiance. SIF radiance is  
 506 significantly higher if wood is neglected in DART simulations, especially in the near-infrared  
 507 domain.  $\varepsilon_{SIF,Lv,NW-W}(\lambda)$  is larger ( $\approx 25\%$ ) at wavelengths above 750nm, and smaller at  
 508 wavelengths smaller than 680nm. This is explained by the fact that there is more multiple  
 509 scattering at these wavelengths, which in turn increases the probability of interception of SIF  
 510 radiation by woody elements.

511

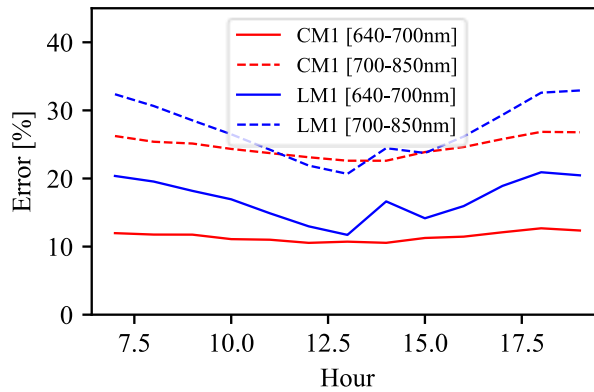


512

513 Figure 16. PSI, PSII and total SIF nadir spectral radiance and error  $\varepsilon_{SIF,Lv,NW-W}(\lambda)$  of 3D CM1 and  
 514 LM1 plots simulated with (W) and without (NW) woody elements at 12.00 (local time)

515 The diurnal relative error of the SIF total nadir radiance for CM1 and LM1 3D plots simulated  
 516 without woody elements, compared to presence of woody elements, varies over the course of  
 517 the day (Figure 17). It is lowest at solar noon for LM1 and relatively stable for CM1. The time  
 518 variability for LM1 is explained by the fact that its leaf and wood densities are in the canopy  
 519 upper layers, which increases the influence of horizontal heterogeneity, and consequently the  
 520 occurrence of smaller errors at noon. Conversely, for CM1, the leaf and wood densities are  
 521 larger at lower tree heights, which leads to smaller horizontal heterogeneity effects, including  
 522 smaller shadow effects.

523

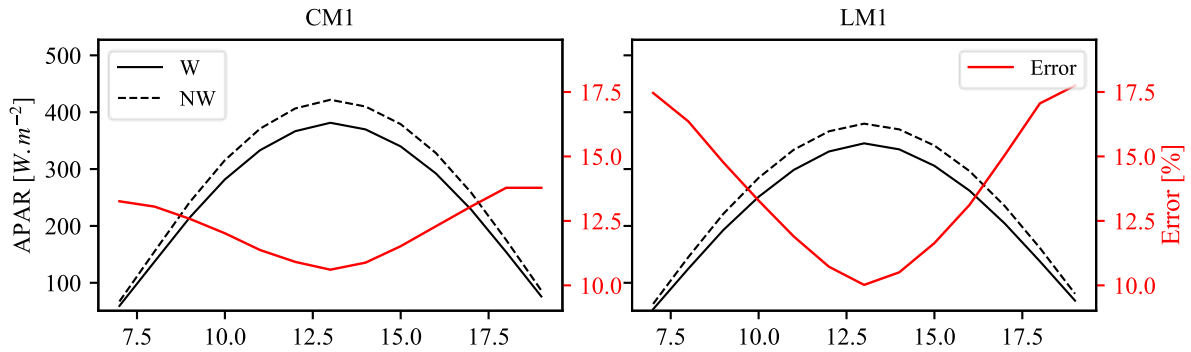


524

525 Figure 17. Diurnal relative error of total nadir SIF radiance  $MARE_{SIF,L_v,NW-W}(t)$  of the CM1 and  
 526 LM1 3D forest plots simulated without woody elements. 640 – 700 nm and 700 – 850 nm.

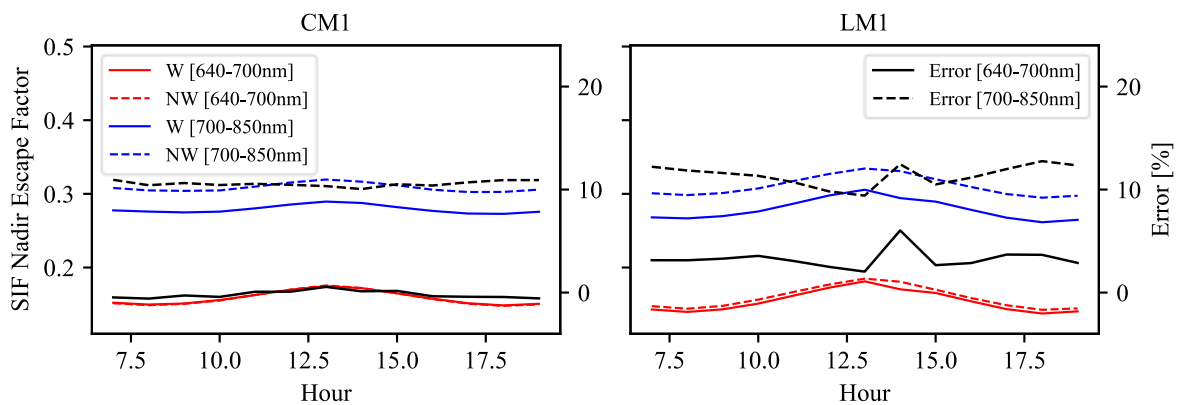
527 The influence of woody elements on the remotely sensed SIF signal can be split into shading  
 528 and blocking effects. These effects are not independent. The shading effect corresponds to the  
 529 shading of leaves by woody elements during the direct sun and atmosphere illumination of the  
 530 forest scene. It limits the absorption of PAR by chlorophylls and consequently decreases leaf  
 531 SIF emission (*i.e.*, 1<sup>st</sup> process). The blocking effect corresponds to the interception (*i.e.*,  
 532 absorption and scattering) by woody elements of SIF radiation from its leaf emission to the exit  
 533 of the forest canopy along the viewing direction of the remote sensing sensor. Figure 18  
 534 illustrates the magnitude of the shading effect. It shows the DART simulated diurnal  
 535  $APAR_{green}(t)$  and the associated relative error  $\varepsilon_{APAR,NW-W}(t)$ , for the CM1 and LM1 3D plots  
 536 with and without woody elements.  $APAR_{green}$  is always larger for the plots without wood, as  
 537 expected. The relative error associated to the shading effect greatly varies over the selected day.  
 538 It is minimal at solar midday, when trunks and branches are blocking the least amount of direct  
 539 solar radiation, and largest in early morning and late afternoon when trunks and branches are  
 540 blocking a larger part of direct PAR. Figure 19 illustrates the blocking effect. It shows the  
 541 diurnal SIF nadir escape factor at [400nm-700nm] and [700nm-850nm] for the CM1 and LM1  
 542 3D plots simulated with (W) and without (NW) woody elements, and the associated relative  
 543 error  $\varepsilon_{SIF.NEF,NW-W}(t)$ . This relative error is nearly constant over the day, conversely to the  
 544 relative error on the canopy  $APAR_{green}$ . Indeed, as a first approximation  $SIF_{nadir EF}$   
 545 corresponds to a quantity that is relatively constant: the sum of the canopy "direct – direct" and  
 546 "diffuse – direct" transmittance (Vermeire et al., 1997) weighted by a normalized vertical  
 547 distribution of leaf SIF emitted radiation. The "diffuse – direct" transmittance is much smaller  
 548 at [640-700nm] than at [700nm-850nm] because vegetation absorbs much more at [640-700nm]  
 549 than at [700nm-850nm]. Since the blocking effect of wood is more pronounced for oblique

550 directions, it has a higher impact on the "diffuse – direct" than on the "direct – direct"  
 551 transmittance. This explains that  $\varepsilon_{SIF,NEF,NW-W}(t)$  is smaller at [640-700nm] than at [700nm-  
 552 850nm].



553

554 Figure 18. Diurnal  $APAR_{green}$  of CM1 and LM1 3D forest plots with (Wood) and without (No Wood)  
 555 woody elements and their associated relative errors  $\varepsilon_{APAR,NW-W}(t)$ .



556

557 Figure 19. Diurnal SIF nadir escape factor over [640nm-700nm] and [700nm-850nm] of CM1 and LM1  
 558 3D plots simulated with (W) and without (NW) woody elements and associated relative error  
 559  $\varepsilon_{SIF,NEF,NW-W}(t)$ .

560

561

## 4. Discussion

562

### 4.1. 3D structure of the forest study sites

563 The comparison of DART simulated SIF and non SIF radiometric quantities of 1D and 3D  
 564 abstractions of the studied forest plots highlights the influence of the forest architecture, and  
 565 especially the forest horizontal heterogeneity, on these quantities:  $APAR_{green}$  ( $\varepsilon_{APAR,1D-3D}(t)$ :  
 566 Figure 8), SIF emitted ( $\varepsilon_{SIF.em,1D-3D}(t)$ : Figure 10), SIF<sub>nadir yield</sub> ( $\varepsilon_{SIF.NY,1D-3D}(t)$ : Figure  
 567 15), canopy SIF exitance and escape factor ( $\varepsilon_{SIF.EF,1D-3D}(t)$ : Figure 12), SIF nadir yield  
 568 ( $\varepsilon_{SIF.NY,1D-3D}(t)$ : Figure 15) and reflectance (Figure 6). Braghieri et al. (2021) found that the

569 SIF modeling was improved by introducing a clumping index (Nilson, 1971; Pinty et al., 2006)  
 570 to replicate the behavior of structurally complex 3D canopies in the 1D model CliMA-Land  
 571 (based on the mSCOPE model (Yang et al., 2017)). In this study, simulating the SIF signal  
 572 while neglecting the forest horizontal heterogeneity can lead to very large relative errors,  
 573 especially for logged “L” forest sites where they can reach 60%. For example, the error on SIF  
 574 radiance  $MARE_{SIF,Lv,1D-3D}(t)$  is higher for the logged “L” forest sites (Figure 5). This is  
 575 consistent with the fact that these forest sites have a higher horizontal heterogeneity, with a  
 576 higher canopy height variability and a higher number of pure bare ground pixels, as shown in  
 577 Table 4 and in the height maps (Figure 2). Generally, the horizontal heterogeneity tends to  
 578 decrease the SIF signal that escapes the forest canopy. The vertical heterogeneity appeared to  
 579 have an opposite effect in most cases. These points are further discussed below.

580

#### 581 **4.2. Effect of 3D architecture on the three processes driving SIF generation**

582 Several sensitivity analysis studies based on radiative transfer modeling were carried out to  
 583 assess the impact of some structural parameters on the SIF such as leaf density, leaf angular  
 584 distribution and fractional vegetation cover (Tong et al., 2021; Zeng et al., 2020), the  
 585 contribution of understory (Hornero et al., 2021), clumping and woody elements impacts  
 586 (Malenovský et al., 2021). In this study, we assessed the impact of canopy heterogeneity on SIF  
 587 and processes driving its generation. High relative errors in nadir SIF radiance were observed  
 588 for the 8 forest plots due to neglecting the 3D forest architecture, in particular, the horizontal  
 589 heterogeneity. Errors were maximal in the hours of the day with lowest PAR having the larger  
 590 shading effects. They were higher than 50% in the most heterogeneous plots (LI2 and LM2)  
 591 and at [640-700nm] where shading effects are higher due to the lower importance of multiple  
 592 scattering in the canopy. The errors in the canopy SIF radiance where forest horizontal  
 593 architecture was neglected (*i.e.*, 1D forest plots) can be explained by two processes that drive  
 594 the SIF signal generation.

595 1)  $APAR_{green}$  is overestimated if the forest horizontal architecture is neglected. It leads to an  
 596 overestimation of the SIF emitted by leaves. This overestimation of SIF emission mainly  
 597 occurs in the upper canopy layers. This is mainly due to the fact that in the forest 1D  
 598 abstractions, the leaves of the top layers are homogeneously distributed, whereas in actual  
 599 3D forests, they can be greatly clumped at two levels: they are grouped within distinct tree

600 crowns, and also, they tend to be clumped within each tree crown. Combined, these effects  
 601 result in upper layers of 1D plots that are more efficiently illuminated than in 3D plots,  
 602 which explains higher SIF emission in 1D plots than in 3D plots. However, in the bottom  
 603 layers, the SIF emission of 1D plots is underestimated. Indeed, the roughness of the actual  
 604 canopy causes a better penetration of light to the bottom layers of the 3D plots, compared  
 605 to the associated 1D plots, where the top layers of the canopy shade more efficiently the  
 606 light. This is illustrated by Figure 11: the profile of SIF emission is similar to the profile of  
 607 LAI with a higher  $\frac{\text{SIF}_{\text{emitted}}}{\text{LAI}}$  value in the top layers. This means that the SIF emission per leaf  
 608 area unit is higher for the top layers because leaves in the top layers are able to capture  
 609 more light than the leaves in the bottom layers.

610 2) The emitted SIF radiation has a higher ability to escape from the canopy in the 1D  
 611 abstractions of the forest plots both for the upward nadir direction (*cf.* SIF yield in Figure  
 612 15), and for the upper hemisphere (*cf.*, SIF escape factor<sub>hemi</sub> in Figure 12). It corresponds  
 613 to an underestimation of the total absorption fraction of SIF in all 1D abstractions of the 8  
 614 forest plots (Table 6, Table 7). This underestimation of SIF absorption is rather large for  
 615 the ground, and larger for [640-700nm] (*i.e.*, between -17 and -43% for [640-700nm],  
 616 between -5% and -35% for [700-850nm]) and rather small for "Leaf + Wood" (*i.e.*, between  
 617 -2 and -4% for [640-700nm], between -1 and -3% for [700-850nm]). LM1 has a slightly  
 618 different behavior: in its 1D abstraction, the absorption of "Leaf + Wood" is slightly  
 619 overestimated for [700-850nm] (*i.e.*, around 2%). Part of the underestimation of SIF  
 620 absorption by the ground for 1D plots is due to the smaller area of the ground in the 1D  
 621 plot compared to the 3D plot where topography is simulated (Table 2).

622 The vertical profiles of SIF emission (Figure 11) and absorption (Figure 14) of the 1D plots  
 623 show that emission and absorption are both overestimated in the top layers and underestimated  
 624 in the bottom layers. A main particularity for the absorption profile is the influence of the  
 625 ground. It shows sharp peaks at 0 m height for 1D simulations. For the 3D abstractions of the  
 626 forest plots, the height of the ground is variable. Therefore, ground absorption peaks appear in  
 627 the bottom for the "C" plots. These peaks are not visible in "L" plots, because of important  
 628 absorption of the leaves and woody elements in the bottom part of the canopies.

629

### 630 **4.3. Influence of 3D architecture on the canopy reflectance.**



631 As a first approximation, SIF emission can be considered as the reflection of radiation at a  
 632 different wavelength from that of the incident radiation. Therefore, it makes sense to find  
 633 similar errors for SIF radiance  $MARE_{SIF,L_v,1D-3D}(t)$  and canopy reflectance  $MARE_{\rho,1D-3D}(t)$ .  
 634 However, SIF has some particularities that may differ from reflectance. Indeed, the SIF  
 635 emission only comes from leaf elements. Other components of the canopy (*i.e.*, woody elements  
 636 and ground) do not emit SIF radiation, even though they contribute indirectly by scattering SIF  
 637 radiation emitted by foliar elements. On the other hand, all elements of the canopy can  
 638 contribute directly to the canopy radiance. Since bare ground does not directly contribute to the  
 639 SIF radiance of forest plots, pure bare ground pixels have SIF radiance values close to zero. A  
 640 nadir viewing sensor cannot see the bare ground in 1D plots, conversely to 3D plots. Hence,  
 641  $MARE_{SIF,L_v,1D-3D}$  tends to be larger than  $MARE_{\rho,1D-3D}$  because for canopy reflectance, pure  
 642 bare ground pixels and vegetation pixels have values of the same order of magnitude. This  
 643 explains that for LI2, the SIF radiance errors (Figure 5) are notably larger than the reflectance  
 644 errors (Figure 7). Indeed, compared to the other sites (cf. Table 4), the LI2 site has the  
 645 particularity to have the largest surface of ground without vegetation cover. Therefore, its  
 646  $MARE_{SIF,L_v,1D-3D}$  tends to be large, especially if the ground reflectance is high. Multiple  
 647 scattering explains that SIF radiance errors are larger in 640 – 700nm than in 700-850nm  
 648 domain. Indeed, in the 700 – 850nm, the shadowing effects due to the canopy structure are  
 649 attenuated by the important multiple scattering in this spectral domain. It is also the case for  
 650 canopy reflectance in most cases expect for LI1 (in the middle of the day) and LI2 (Figure 7).  
 651 This is because we only consider the 640 – 700nm spectral region and not all the 400 – 700nm  
 652 for the comparison with SIF. Indeed, In Figure 6, we see that for these plots,  $\varepsilon_{\rho,1D-3D}(\lambda)$  has a  
 653 local minimum around 680nm, and even a sign change for LI2.

654

#### 655 **4.4. Influence of woody elements**

656 Although woody elements do not generate SIF emission, their interaction with the  
 657 photosynthetically active light and with SIF radiation emitted by leaves can highly impact the  
 658 SIF signal, as shown in (Malenovský et al., 2021). We studied their influence on the SIF signal  
 659 by comparing the SIF signal of forest plots that was simulated without and with woody elements.  
 660 For that, we removed the woody elements from the 3D abstractions of the CM1 and LM1 plots.  
 661 It appeared that the plots without woody elements had a higher simulated SIF radiance,

662 especially in the 700-850 nm spectral domain where multiple scattering is highly influenced by  
 663 the presence of woody elements. The influence of woody elements is smaller in the 640 – 700  
 664 nm spectral domain. The shading effect of woody elements on SIF emission leads to a lower  
 665  $fAPAR_{green}$  (Figure 18) and therefore triggering less SIF emission. It was shown to be more  
 666 important than the blocking effect of woody elements (Figure 19), especially for oblique solar  
 667 directions and at 640-700 nm.

668

## 669 5. Concluding remarks

670 This study investigated the potential effect of the forest 3D architecture on diurnal nadir SIF  
 671 RS observations and SIF emissions inside the canopy. We studied the following three processes  
 672 responsible for modulation of the canopy SIF signal: i) the attenuation of incident PAR in the  
 673 canopy, ii) the leaf SIF emission efficiency, and iii) the attenuation of the SIF between its place  
 674 of emission and its observation above the canopy. The potential impact of woody elements on  
 675 the SIF signal of forest stands was also investigated. Eight study sites, located within the  
 676 temperate deciduous forest in the Smithsonian Environmental Research Center, were modeled  
 677 using the DART-FT and DART-Lux radiative transfer modes and the effects of their forest  
 678 architecture were assessed by comparing SIF quantities of the sites simulated as 3D, 1D and  
 679 0D scenes.

680 Although several general trends common to all sites were clearly identified, some results  
 681 were of the site-specific nature due to structural differences in canopy horizontal and vertical  
 682 heterogeneity. Results revealed that the horizontal heterogeneity of forests had a larger  
 683 influence than the canopy vertical heterogeneity. Therefore, for a correct modeling of remotely  
 684 sensed SIF signals of spatially heterogeneous canopies, one must consider the full 3D  
 685 architecture of forests and not only their vertical heterogeneity as being assumed in 1D RTMs.

686 Studying the propagation of SIF radiation within the canopy through quantitative  
 687 parameters, such as the SIF escape factor and the nadir SIF yield, is essential for linking the  
 688 SIF RS observation to the canopy foliage SIF emission. Three key indicators were able to  
 689 explain most of the differences between the nadir SIF signal of canopies simulated as 3D and  
 690 1D landscapes. The SIF escape factor ( $\epsilon_{1D-3D}$  up to 40%) was shown to be the most indicative  
 691 parameter, followed by the attenuation of incident PAR and consequently reduction of  
 692  $fAPAR_{green}$  ( $\epsilon_{1D-3D}$  less than 5%), and the SIF emission yield ( $\epsilon_{1D-3D}$  less than 2%) induced  
 693 by different  $f_{qe}$  values assigned to the sun- and shade-adapted leaves. Our results indicated that

694 the influence of forest architecture on SIF escape factor and nadir SIF yield values ( $\epsilon$  up to 40%)  
695 varies in time, with differences in forest stand structure and per spectral domain, with  $\epsilon$  being  
696 always greater for the wavelength range of 640 – 700 nm than for the range of 700 – 850 nm.

697 The presence of woody elements inside DART-simulated forest scenes appeared to have  
698 a relatively large influence on the canopy SIF radiance through the two effects: i) a shading of  
699 photosynthetically active foliage and ii) a blocking (obstruction) of SIF radiation. The relative  
700 error associated with the neglect of wood existence ranged between 10% and 35%,  
701 depending on analyzed spectral domain and forest site, where the relative errors for the shading  
702 effect were ranging between 10 and 20%, and for the blocking effect between 0 and 10%.

703 Although this work underlines the usefulness of 3D RTMs for investigating physical  
704 bases linking RS SIF observations with SIF emitted inside a forest canopy, there are several  
705 modeling aspects that should be reconsidered and improved in the follow-up work. For example,  
706 leaf SIF emission properties were assumed to be constant throughout the day, *i.e.*, the actual  
707 modulation of SIF emission by local environmental conditions (*e.g.*, leaf temperature, air  
708 humidity, etc.) was not considered. Remediation of this strong assumption requires inclusion of  
709 a full canopy energy balance in the DART modeling scheme, that would allow to account for  
710 crucial environmental parameters of radiative (*i.e.*, visible, near infrared and thermal infrared  
711 radiation budgets) as well as non-radiative processes (*e.g.*, photosynthesis). This is currently  
712 possible only by coupling DART with a 1D energy budget model like SCOPE. The development  
713 of a 3D energy balance modeling, based on DART radiation budget computations, is on the list  
714 of our future works. Three major DART-Lux modeling works, partly completed, will also be very  
715 helpful for rapid simulations of SIF over larger landscapes: SIF and thermal emission of  
716 vegetation simulated as turbid medium, and 3D radiative budget, including SIF emission.

717

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 727 providing leaf biochemical properties measured for the selected SERC forest species and her  
 728 contribution to the improvement of the manuscript.

729

### 730 **Appendix 1: Conversion of turbid voxels into triangles clouds.**

731 Each turbid cell of a forest mock-ups is converted to a linear combination of a few 3D objects  
 732 (i.e., made of facets) among N cell objects whose LAI is  $LAI_n$ , with  $n \in [1 N]$ . Accuracy on the  
 733 simulated LAI is  $10^{-2}$  with  $N = 16$  with  $LAI_n$  equal to 0.01, 0.02, 0.05, 0.1, 0.2, 0.3, 0.4, 0.5, 1, 1.5,  
 734 2, 2.5, 3, 3.5, 4, and 4.5. The area of a facet in each cell object is  $5 \cdot 10^{-5} \text{ m}^2$  if  $LAI_n \leq 2$ , and  $10^{-4}$   
 735  $\text{m}^2$  if  $LAI_n > 2$ .

736

737 The algorithm of the conversion method is based on the value of  $LAI_{cell}$  of the turbid cell to  
 738 convert:

739 \* Scene  $LAI_{cell} < 1$ : the turbid cell is replaced by two 3D cell objects at most:

740 - 1<sup>st</sup> cell object (i.e., cell object with the larger LAI): it can be only enlarged. Its enlargement  
 741 is 5% at most. If it should be 5% to get the exact LAI of the turbid cell, then a 2<sup>nd</sup> cell is  
 742 introduced.

743 - 2<sup>nd</sup> cell object: it can be enlarged or shrunk.

744 \* Scene  $LAI_{cell} > 1$ : the turbid cell is replaced by three cell objects cells at most:

745 - 1<sup>st</sup> cell object: it cannot be scaled. If precision  $< 10^{-2}$ , then a 2<sup>nd</sup> cell is used.

746 - 2<sup>nd</sup> cell object: it can be only enlarged, by 5% at most. A 3<sup>rd</sup> cell is used if a larger  
 747 enlargement is needed.

748 - 3<sup>rd</sup> cell object: it can be enlarged or shrunk.

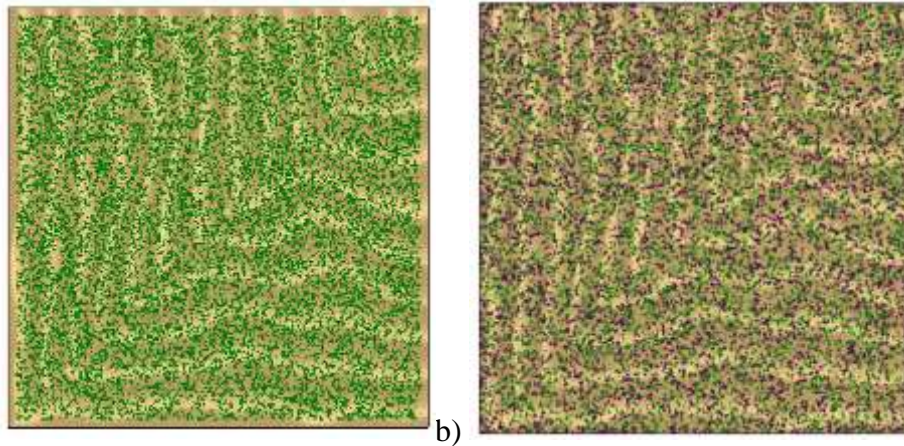
#### 749 Examples of replacement of a turbid cell ( $LAI_{cell}$ ) by up to 3 3D cell objects:

750 -  $LAI_{cell} = 0.92$  (Figure 20). Replacing it by a cell object of  $LAI = 1$ , (i.e., shrinking it by a factor  
 751 0.96) would create 2 cm wide empty spaces at the cell borders. Therefore, it was instead replaced  
 752 by a cell object of  $LAI = 0.5$  and a cell object of  $LAI = 0.4$  enlarged by a factor 1.025. (i.e.,  $0.92$   
 753  $\approx 0.5 + 0.4 \times 1.025^2$ ).

754 -  $LAI_{cell} = 0.23 (\approx 0.2 + 0.02 \times 1.2247^2) \Rightarrow$  2 cell objects:  $LAI_n = 0.2$ ,  $LAI_n = 0.02$  scaled by 1.2247

755 -  $LAI_{cell} = 0.48 (\approx 0.4 + 0.1 \times 0.8944^2) \Rightarrow$  2 cell objects:  $LAI_n = 0.4$ ,  $LAI_n = 0.1$  shrunk by 0.8944

- 756 -  $LAI_{cell} = 0.93 (\approx 0.5 + 0.4 \times 1.0368^2) \Rightarrow$  2 cell objects:  $LAI_n=0.5$ ,  $LAI_n=0.4$  scaled by 1.0368  
 757 -  $LAI_{cell} = 0.64 (\approx 0.5 + 0.1 + 0.05 \times 0.8944) \Rightarrow$  3 cell objects:  $LAI_n=0.5$ ,  $LAI_n=0.1$ ,  $LAI_n=0.05$   
 758     shrunk by 0.8944.  
 759  
 760



761     a)     b)  
 762 Figure 20. Top view of a turbid cell of  $LAI = 0.92$  simulated with  $N$  cell objects. a)  $N=1$ : cell  
 763 object of  $LAI = 1$  is shrunk by a factor 0.96, resulting in empty space along the borders of the  
 764 cell. b)  $N=2$ : 3D object of  $LAI = 0.5$  (green) + 3D object of  $LAI = 0.4$  enlarged by a factor  
 765 1.025 (purple).  
 766

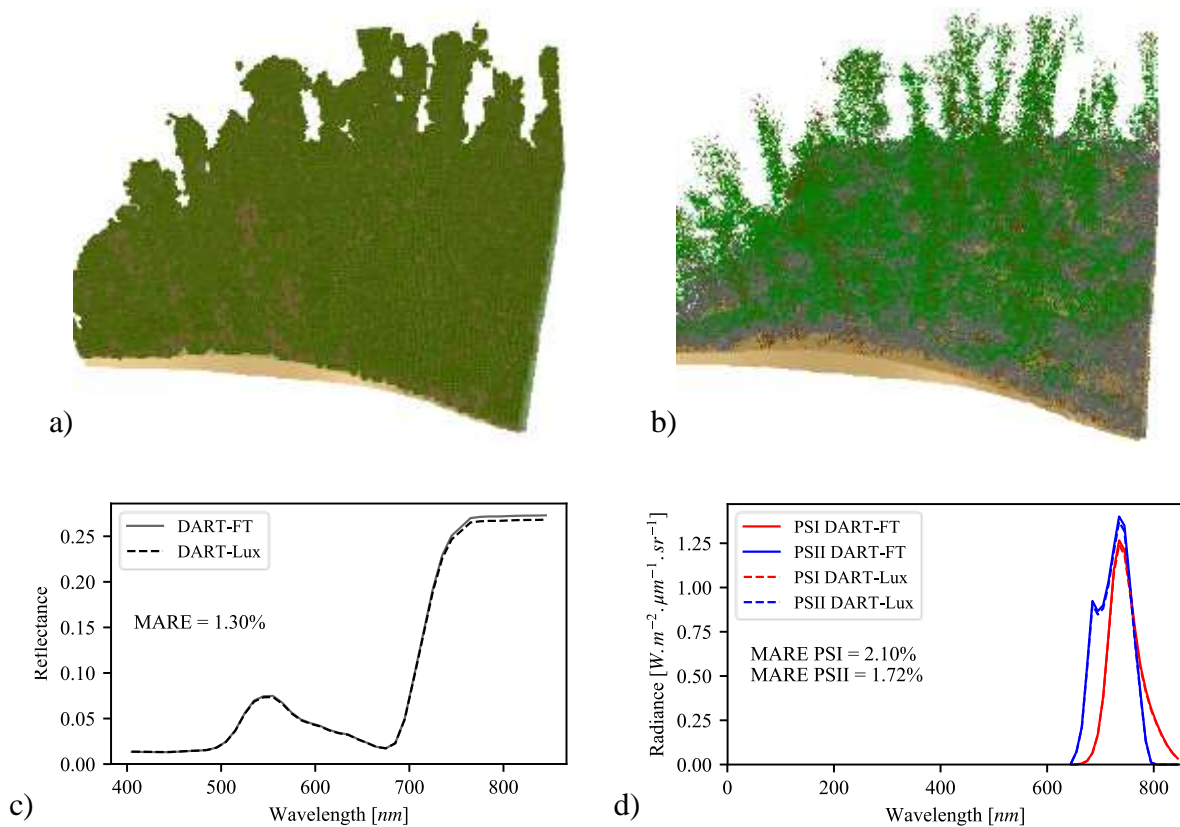
767 This conversion method ensures that the mock-up is represented by a finite number of 3D objects  
 768 (i.e.,  $16 \times 3 = 48$ ). It also avoids the appearance of holes due to shrinking the 3D objects, and large  
 769 exceeding of voxel limits due to the enlargement of 3D objects.  $M=3$  samples of each cell object  
 770 are randomly used to introduce a random variability in the mock-ups. Also, a random rotation of  
 771  $0^\circ$ ,  $90^\circ$ ,  $180^\circ$  or  $270^\circ$  relative to the vertical axis ensures more randomness of the simulated cell.

772

### 773 **Appendix 2: Equivalence between DART-FT and DART-Lux simulations**

774 Our work combines DART-FT simulations of radiative budget and DART-Lux simulations of  
 775 scene radiance / reflectance. Therefore, the consistency of these two DART modes is an essential  
 776 point. Relative differences of DART-FT and DART-Lux can be as small as  $10^{-5}$  depending on  
 777 their modeling parameters of each mode. For example, the number of discrete directions for  
 778 DART-FT, and the number of samples per pixel for DART-Lux. Here, this similarity is illustrated

779 through the comparison of the reflectance and SIF radiance of LM1, using model parameters hat  
 780 were used in our work. Figure 21 indicates that MARE is equal to 1.3% for scene reflectance,  
 781 2.1% for PSI radiance, and 1.72% for PSII radiance.



782  
 783 Figure 21: Comparison of DART-FT (turbid voxels) and DART-Lux (turbid voxels transformed to  
 784 triangles) for a 10m x 10m subscene of CI1. a) LM1 turbid mock-up. b) LM1 triangles cloud  
 785 mock-up (after conversion). Green: sun-adapted leaves, Grey: shade-adapted leaves, Brown:  
 786 woody elements. c) DART-FT and DART-Lux scene reflectance. d) Scene PSI and PSII  
 787 radiance simulated by DART-FT and DART-Lux.

788

789 **References**

- 790 Ač, A., Malenovský, Z., Olejníčková, J., Gallé, A., Rascher, U., & Mohammed, G. (2015).  
 791 Meta-analysis assessing potential of steady-state chlorophyll fluorescence for remote  
 792 sensing detection of plant water, temperature and nitrogen stress. *Remote Sensing of*  
 793 *Environment*, 168, 420–436. <https://doi.org/10.1016/j.rse.2015.07.022>
- 794 Baker, N. R. (2008). Chlorophyll Fluorescence: A Probe of Photosynthesis In Vivo. *Annual*  
 795 *Review of Plant Biology*, 59(1), 89–113.  
 796 <https://doi.org/10.1146/annurev.arplant.59.032607.092759>
- 797 Braghieri, R. K., Wang, Y., Doughty, R., Sousa, D., Magney, T., Widlowski, J.-L., Longo,  
 798 M., Bloom, A. A., Worden, J., Gentine, P., & Frankenberg, C. (2021). Accounting for  
 799 canopy structure improves hyperspectral radiative transfer and sun-induced  
 800 chlorophyll fluorescence representations in a new generation Earth System model.  
 801 *Remote Sensing of Environment*, 261, 112497.  
 802 <https://doi.org/10.1016/j.rse.2021.112497>
- 803 Brede, B., Verrelst, J., Gastellu-Etchegorry, J.-P., Clevers, J. G. P. W., Goudzwaard, L., den  
 804 Ouden, J., Verbesselt, J., & Herold, M. (2020). Assessment of Workflow Feature  
 805 Selection on Forest LAI Prediction with Sentinel-2A MSI, Landsat 7 ETM+ and  
 806 Landsat 8 OLI. *Remote Sensing*, 12(6), Article 6. <https://doi.org/10.3390/rs12060915>
- 807 Campbell, P. K. E., Huemmrich, K. F., Middleton, E. M., Ward, L. A., Julitta, T., Daughtry,  
 808 C. S. T., Burkart, A., Russ, A. L., & Kustas, W. P. (2019). Diurnal and Seasonal  
 809 Variations in Chlorophyll Fluorescence Associated with Photosynthesis at Leaf and  
 810 Canopy Scales. *Remote Sensing*, 11(5), Article 5. <https://doi.org/10.3390/rs11050488>
- 811 Campbell, P. K. E., Middleton, E. M., McMurtrey, J. E., Corp, L. A., & Chappelle, E. W.  
 812 (2007). Assessment of vegetation stress using reflectance or fluorescence  
 813 measurements. *Journal of Environmental Quality*, 36(3), 832–845.  
 814 <https://doi.org/10.2134/jeq2005.0396>
- 815 Campbell, P. K. E., Ward, L. A., Huemmrich, K. F., & Middleton, E. (2018). Diurnal and  
 816 seasonal dynamics in chlorophyll fluorescence, xanthophyll cycle and photosynthetic  
 817 function, at leaf and canopy scales. *AGU Fall Meeting Abstracts*, 33.  
 818 <http://adsabs.harvard.edu/abs/2018AGUFM.B33C..07C>

- 819 Cook, B. D., Corp, L. A., Nelson, R. F., Middleton, E. M., Morton, D. C., McCorkel, J. T.,  
 820 Masek, J. G., Ranson, K. J., Ly, V., & Montesano, P. M. (2013). NASA Goddard's  
 821 LiDAR, Hyperspectral and Thermal (G-LiHT) Airborne Imager. *Remote Sensing*,  
 822 5(8), Article 8. <https://doi.org/10.3390/rs5084045>
- 823 Damm, A., Guanter, L., Paul-Limages, E., Tol, C. van der, Hueni, A., Buchmann, N., Eugster,  
 824 W., Ammann, C., & Schaepman, M. E. (2015). Far-red sun-induced chlorophyll  
 825 fluorescence shows ecosystem - specific relationships to gross primary production: An  
 826 assessment based on observational and modeling approaches. *Remote Sensing of*  
 827 *Environment*, 166, 91–105. <https://doi.org/10.1016/j.rse.2015.06.004>
- 828 Drusch, M., Moreno, J., Bello, U. D., Franco, R., Goulas, Y., Huth, A., Kraft, S., Middleton,  
 829 E. M., Miglietta, F., Mohammed, G., Nedbal, L., Rascher, U., Schüttemeyer, D., &  
 830 Verhoef, W. (2017). The FLuorescence EXplorer Mission Concept—ESA's Earth  
 831 Explorer 8. *IEEE Transactions on Geoscience and Remote Sensing*, 55(3), 1273–1284.  
 832 <https://doi.org/10.1109/TGRS.2016.2621820>
- 833 Fournier, A., Daumard, F., Champagne, S., Ounis, A., Goulas, Y., & Moya, I. (2012). Effect  
 834 of canopy structure on sun-induced chlorophyll fluorescence. *ISPRS Journal of*  
 835 *Photogrammetry and Remote Sensing*, 68, 112–120.  
 836 <https://doi.org/10.1016/j.isprsjprs.2012.01.003>
- 837 Gastellu-Etchegorry, J.-P., Demarez, V., Pinel, V., & Zagolski, F. (1996). Modeling radiative  
 838 transfer in heterogeneous 3-D vegetation canopies. *Remote Sensing of Environment*,  
 839 58(2), 131–156. [https://doi.org/10.1016/0034-4257\(95\)00253-7](https://doi.org/10.1016/0034-4257(95)00253-7)
- 840 Gastellu-Etchegorry, J.-P., Lauret, N., Yin, T., Landier, L., Kallel, A., Malenovský, Z., Bitar,  
 841 A. A., Aval, J., Benhmida, S., Qi, J., Medjdoub, G., Guilleux, J., Chavanon, E., Cook,  
 842 B., Morton, D., Chrysoulakis, N., & Mitraka, Z. (2017). DART: Recent Advances in  
 843 Remote Sensing Data Modeling With Atmosphere, Polarization, and Chlorophyll  
 844 Fluorescence. *IEEE Journal of Selected Topics in Applied Earth Observations and*  
 845 *Remote Sensing*, 10(6), 2640–2649. <https://doi.org/10.1109/JSTARS.2017.2685528>
- 846 Gastellu-Etchegorry, J.-P., Yin, T., Lauret, N., Cajgfinger, T., Gregoire, T., Grau, E., Feret, J.-  
 847 B., Lopes, M., Guilleux, J., Dedieu, G., Malenovský, Z., Cook, B. D., Morton, D.,  
 848 Rubio, J., Durrieu, S., Cazanave, G., Martin, E., & Ristorcelli, T. (2015). Discrete  
 849 Anisotropic Radiative Transfer (DART 5) for Modeling Airborne and Satellite



## CHAPTER 4: IMPACT OF VEGETATION 3D STRUCTURE ON SIF

- 850 Spectroradiometer and LIDAR Acquisitions of Natural and Urban Landscapes.  
851 *Remote Sensing*, 7(2), Article 2. <https://doi.org/10.3390/rs70201667>
- 852 Gastellu-Etchegorry, J.-P., Yin, T., Lauret, N., Grau, E., Rubio, J., Cook, B. D., Morton, D.  
853 C., & Sun, G. (2016). Simulation of satellite, airborne and terrestrial LiDAR with  
854 DART (I): Waveform simulation with quasi-Monte Carlo ray tracing. *Remote Sensing*  
855 *of Environment*, 184, 418–435. <https://doi.org/10.1016/j.rse.2016.07.010>
- 856 Georgiev, I., Krivánek, J., Davidovič, T., & Slusallek, P. (2012). Light transport simulation  
857 with vertex connection and merging. *ACM Transactions on Graphics*, 31(6), 192:1-  
858 192:10. <https://doi.org/10.1145/2366145.2366211>
- 859 Givnish, T. J. (1988). Adaptation to Sun and Shade: A Whole-Plant Perspective. *Functional*  
860 *Plant Biology*, 15(2), 63–92. <https://doi.org/10.1071/pp9880063>
- 861 Guanter, L., Zhang, Y., Jung, M., Joiner, J., Voigt, M., Berry, J. A., Frankenberg, C., Huete,  
862 A. R., Zarco-Tejada, P., Lee, J.-E., Moran, M. S., Ponce-Campos, G., Beer, C.,  
863 Camps-Valls, G., Buchmann, N., Gianelle, D., Klumpp, K., Cescatti, A., Baker, J. M.,  
864 & Griffis, T. J. (2014). Global and time-resolved monitoring of crop photosynthesis  
865 with chlorophyll fluorescence. *Proceedings of the National Academy of Sciences*,  
866 111(14), E1327–E1333. <https://doi.org/10.1073/pnas.1320008111>
- 867 Hernández-Clemente, R., North, P. R. J., Hornero, A., & Zarco-Tejada, P. J. (2017).  
868 Assessing the effects of forest health on sun-induced chlorophyll fluorescence using  
869 the FluorFLIGHT 3-D radiative transfer model to account for forest structure. *Remote*  
870 *Sensing of Environment*, 193, 165–179. <https://doi.org/10.1016/j.rse.2017.02.012>
- 871 Hornero, A., North, P. R. J., Zarco-Tejada, P. J., Rascher, U., Martín, M. P., Migliavacca, M.,  
872 & Hernandez-Clemente, R. (2021). Assessing the contribution of understory sun-  
873 induced chlorophyll fluorescence through 3-D radiative transfer modelling and field  
874 data. *Remote Sensing of Environment*, 253, 112195.  
875 <https://doi.org/10.1016/j.rse.2020.112195>
- 876 Kallel, A. (2020). FluLCVRT: Reflectance and fluorescence of leaf and canopy modeling  
877 based on Monte Carlo vector radiative transfer simulation. *Journal of Quantitative*  
878 *Spectroscopy and Radiative Transfer*, 253, 107183.  
879 <https://doi.org/10.1016/j.jqsrt.2020.107183>

- 880 Kamoske, A. G., Dahlin, K. M., Stark, S. C., & Serbin, S. P. (2019). Leaf area density from  
881 airborne LiDAR: Comparing sensors and resolutions in a temperate broadleaf forest  
882 ecosystem. *Forest Ecology and Management*, 433, 364–375.  
883 <https://doi.org/10.1016/j.foreco.2018.11.017>
- 884 Kobayashi, H., & Iwabuchi, H. (2008). A coupled 1-D atmosphere and 3-D canopy radiative  
885 transfer model for canopy reflectance, light environment, and photosynthesis  
886 simulation in a heterogeneous landscape. *Remote Sensing of Environment*, 112(1),  
887 173–185. <https://doi.org/10.1016/j.rse.2007.04.010>
- 888 Liu, W., Atherton, J., Möttus, M., Gastellu-Etchegorry, J.-P., Malenovský, Z., Raunonen, P.,  
889 Åkerblom, M., Mäkipää, R., & Porcar-Castell, A. (2019). Simulating solar-induced  
890 chlorophyll fluorescence in a boreal forest stand reconstructed from terrestrial laser  
891 scanning measurements. *Remote Sensing of Environment*, 232, 111274.  
892 <https://doi.org/10.1016/j.rse.2019.111274>
- 893 Liu, W., Luo, S., Lu, X., Atherton, J., & Gastellu-Etchegorry, J.-P. (2020). Simulation-Based  
894 Evaluation of the Estimation Methods of Far-Red Solar-Induced Chlorophyll  
895 Fluorescence Escape Probability in Discontinuous Forest Canopies. *Remote Sensing*,  
896 12(23), Article 23. <https://doi.org/10.3390/rs12233962>
- 897 Liu, X., Guanter, L., Liu, L., Damm, A., Malenovský, Z., Rascher, U., Peng, D., Du, S., &  
898 Gastellu-Etchegorry, J.-P. (2019). Downscaling of solar-induced chlorophyll  
899 fluorescence from canopy level to photosystem level using a random forest model.  
900 *Remote Sensing of Environment*, 231, 110772.  
901 <https://doi.org/10.1016/j.rse.2018.05.035>
- 902 Liu, Z., Lu, X., An, S., Heskell, M., Yang, H., & Tang, J. (2019). Advantage of multi-band  
903 solar-induced chlorophyll fluorescence to derive canopy photosynthesis in a temperate  
904 forest. *Agricultural and Forest Meteorology*, 279, 107691.  
905 <https://doi.org/10.1016/j.agrformet.2019.107691>
- 906 *LuxCoreRender – Open Source Physically Based Renderer*. (n.d.). Retrieved March 29, 2021,  
907 from <https://luxcorerender.org/>
- 908 Malenovský, Z., Martin, E., Homolová, L., Gastellu-Etchegorry, J. P., Zurita-Milla, R.,  
909 Schaepman, M. E., Polorný, R., Clevers, J. G. P. W., & Cudlín, P. (2008). Influence of

## CHAPTER 4: IMPACT OF VEGETATION 3D STRUCTURE ON SIF

- 910 woody elements of a Norway spruce canopy on nadir reflectance simulated by the  
911 DART model at very high spatial resolution. *Remote Sensing of Environment*, 112(1),  
912 1–18. <https://doi.org/10.1016/j.rse.2006.02.028>
- 913 Malenovský, Z., Regaieg, O., Yin, T., Lauret, N., Guilleux, J., Chavanon, E., Duran, N.,  
914 Janoutová, R., Delavois, A., Meynier, J., Medjdoub, G., Yang, P., Van der Tol, C.,  
915 Morton, D., Cook, B., & Gastellu-Etchegorry, J. P. (2021). Discrete Anisotropic  
916 Radiative Transfer Modelling of Solar-induced Chlorophyll Fluorescence: Structural  
917 Impacts in Geometrically Explicit Vegetation Canopies. *Remote Sensing of*  
918 *Environment*.
- 919 Meroni, M., Rossini, M., Guanter, L., Alonso, L., Rascher, U., Colombo, R., & Moreno, J.  
920 (2009). Remote sensing of solar-induced chlorophyll fluorescence: Review of methods  
921 and applications. *Remote Sensing of Environment*, 113(10), 2037–2051.  
922 <https://doi.org/10.1016/j.rse.2009.05.003>
- 923 Migliavacca, M., Perez-Priego, O., Rossini, M., El-Madany, T. S., Moreno, G., Tol, C. van  
924 der, Rascher, U., Berninger, A., Bessenbacher, V., Burkart, A., Carrara, A., Fava, F.,  
925 Guan, J.-H., Hammer, T. W., Henkel, K., Juarez-Alcalde, E., Julitta, T., Kolle, O.,  
926 Martín, M. P., ... Reichstein, M. (2017). Plant functional traits and canopy structure  
927 control the relationship between photosynthetic CO<sub>2</sub> uptake and far-red sun-induced  
928 fluorescence in a Mediterranean grassland under different nutrient availability. *New*  
929 *Phytologist*, 214(3), 1078–1091. <https://doi.org/10.1111/nph.14437>
- 930 Mohammed, G. H., Colombo, R., Middleton, E. M., Rascher, U., van der Tol, C., Nedbal, L.,  
931 Goulas, Y., Pérez-Priego, O., Damm, A., Meroni, M., Joiner, J., Cogliati, S., Verhoef,  
932 W., Malenovský, Z., Gastellu-Etchegorry, J.-P., Miller, J. R., Guanter, L., Moreno, J.,  
933 Moya, I., ... Zarco-Tejada, P. J. (2019). Remote sensing of solar-induced chlorophyll  
934 fluorescence (SIF) in vegetation: 50 years of progress. *Remote Sensing of*  
935 *Environment*, 231, 111177. <https://doi.org/10.1016/j.rse.2019.04.030>
- 936 Nilson, T. (1971). A theoretical analysis of the frequency of gaps in plant stands. *Agricultural*  
937 *Meteorology*, 8, 25–38. [https://doi.org/10.1016/0002-1571\(71\)90092-6](https://doi.org/10.1016/0002-1571(71)90092-6)
- 938 Nobel, P. S. (1976). Photosynthetic Rates of Sun versus Shade Leaves of *Hyptis emoryi* Torr.  
939 *Plant Physiology*, 58(2), 218–223. <https://doi.org/10.1104/pp.58.2.218>

- 940 North, P. R. J. (1996). Three-dimensional forest light interaction model using a Monte Carlo  
 941 method. *IEEE Transactions on Geoscience and Remote Sensing*, 34(4), 946–956.  
 942 <https://doi.org/10.1109/36.508411>
- 943 Parker, G. G. (1995). Structure and microclimate of forest canopies. *Forest Canopies.*, 73–  
 944 106.
- 945 Pinty, B., Lavergne, T., Dickinson, R. E., Widlowski, J.-L., Gobron, N., & Verstraete, M. M.  
 946 (2006). Simplifying the interaction of land surfaces with radiation for relating remote  
 947 sensing products to climate models. *Journal of Geophysical Research: Atmospheres*,  
 948 111(D2). <https://doi.org/10.1029/2005JD005952>
- 949 Regaieg, O., Wang, Y., Malenovský, Z., Yin, T., Kallel, A., Duran, N., Delavois, A., Qi, J.,  
 950 Chavanon, E., Lauret, N., Guilleux, J., Cook, B., Morton, D., & Gastellu-Etchegorry,  
 951 J. P. (2020). Simulation of Solar-Induced Chlorophyll Fluorescence from 3D Canopies  
 952 with the Dart Model. *IGARSS 2020 - 2020 IEEE International Geoscience and*  
 953 *Remote Sensing Symposium*, 4846–4849.  
 954 <https://doi.org/10.1109/IGARSS39084.2020.9323616>
- 955 Rossini, M., Nedbal, L., Guanter, L., Ač, A., Alonso, L., Burkart, A., Cogliati, S., Colombo,  
 956 R., Damm, A., Drusch, M., Hanus, J., Janoutova, R., Julitta, T., Kokkalis, P., Moreno,  
 957 J., Novotny, J., Panigada, C., Pinto, F., Schickling, A., ... Rascher, U. (2015). Red and  
 958 far red Sun-induced chlorophyll fluorescence as a measure of plant photosynthesis.  
 959 *Geophysical Research Letters*, 42(6), 1632–1639.  
 960 <https://doi.org/10.1002/2014GL062943>
- 961 Sakai, Y., Kobayashi, H., & Kato, T. (2020). FLiES-SIF version 1.0: Three-dimensional  
 962 radiative transfer model for estimating solar induced fluorescence. *Geoscientific*  
 963 *Model Development*, 13(9), 4041–4066. <https://doi.org/10.5194/gmd-13-4041-2020>
- 964 Tong, C., Bao, Y., Zhao, F., Fan, C., Li, Z., & Huang, Q. (2021). Evaluation of the FluorWPS  
 965 Model and Study of the Parameter Sensitivity for Simulating Solar-Induced  
 966 Chlorophyll Fluorescence. *Remote Sensing*, 13(6), Article 6.  
 967 <https://doi.org/10.3390/rs13061091>
- 968 van der Tol, C., Verhoef, W., Timmermans, J., Verhoef, A., & Su, Z. (2009). An integrated  
 969 model of soil-canopy spectral radiances, photosynthesis, fluorescence, temperature

## CHAPTER 4: IMPACT OF VEGETATION 3D STRUCTURE ON SIF

- 970 and energy balance. *Biogeosciences*, 6(12), 3109–3129. [https://doi.org/10.5194/bg-6-](https://doi.org/10.5194/bg-6-3109-2009)  
971 3109-2009
- 972 van der Tol, C., Vilfan, N., Dauwe, D., Cendrero-Mateo, M. P., & Yang, P. (2019). The  
973 scattering and re-absorption of red and near-infrared chlorophyll fluorescence in the  
974 models Fluspect and SCOPE. *Remote Sensing of Environment*, 232, 111292.  
975 <https://doi.org/10.1016/j.rse.2019.111292>
- 976 Verhoef, W. (1984). Light scattering by leaf layers with application to canopy reflectance  
977 modeling: The SAIL model. *Remote Sensing of Environment*, 16(2), 125–141.  
978 [https://doi.org/10.1016/0034-4257\(84\)90057-9](https://doi.org/10.1016/0034-4257(84)90057-9)
- 979 Vermote, E., Tanré, D., Deuze, J., Herman, M., & Morcette, J.-J. (1997). Second Simulation  
980 of the Satellite Signal in the Solar Spectrum, 6S: An overview. *IEEE Trans. Geosci.*  
981 *Remote. Sens.* <https://doi.org/10.1109/36.581987>
- 982 Verrelst, J., Malenovsky, Z., Tol, C. van der, Camps-Valls, G., Gastellu-Etchegorry, J.-P.,  
983 Lewis, P., North, P., & Moreno, J. (2019). Quantifying Vegetation Biophysical  
984 Variables from Imaging Spectroscopy Data: A Review on Retrieval Methods. *Surveys*  
985 *in Geophysics*, 40(3), 589–629. <https://doi.org/10.1007/s10712-018-9478-y>
- 986 Verrelst, J., Rivera, J. P., van der Tol, C., Magnani, F., Mohammed, G., & Moreno, J. (2015).  
987 Global sensitivity analysis of the SCOPE model: What drives simulated canopy-  
988 leaving sun-induced fluorescence? *Remote Sensing of Environment*, 166, 8–21.  
989 <https://doi.org/10.1016/j.rse.2015.06.002>
- 990 Verrelst, J., van der Tol, C., Magnani, F., Sabater, N., Rivera, J. P., Mohammed, G., &  
991 Moreno, J. (2016). Evaluating the predictive power of sun-induced chlorophyll  
992 fluorescence to estimate net photosynthesis of vegetation canopies: A SCOPE  
993 modeling study. *Remote Sensing of Environment*, 176, 139–151.  
994 <https://doi.org/10.1016/j.rse.2016.01.018>
- 995 Vilfan, N., van der Tol, C., Muller, O., Rascher, U., & Verhoef, W. (2016). Fluspect-B: A  
996 model for leaf fluorescence, reflectance and transmittance spectra. *Remote Sensing of*  
997 *Environment*, 186, 596–615. <https://doi.org/10.1016/j.rse.2016.09.017>
- 998 Vilfan, N., Van der Tol, C., Yang, P., Wyber, R., Malenovský, Z., Robinson, S. A., &  
999 Verhoef, W. (2018). Extending Fluspect to simulate xanthophyll driven leaf

- 1000 reflectance dynamics. *Remote Sensing of Environment*, 211, 345–356.  
 1001 <https://doi.org/10.1016/j.rse.2018.04.012>
- 1002 Wang, Y., & Gastellu-Etchegorry, J.-P. (2021). Accurate and fast simulation of remote  
 1003 sensing images at top of atmosphere with DART-Lux. *Remote Sensing of*  
 1004 *Environment*, 256, 112311. <https://doi.org/10.1016/j.rse.2021.112311>
- 1005 Wellburn, A. R. (1994). The Spectral Determination of Chlorophylls a and b, as well as Total  
 1006 Carotenoids, Using Various Solvents with Spectrophotometers of Different  
 1007 Resolution. *Journal of Plant Physiology*, 144(3), 307–313.  
 1008 [https://doi.org/10.1016/S0176-1617\(11\)81192-2](https://doi.org/10.1016/S0176-1617(11)81192-2)
- 1009 Yang, P., van der Tol, C., Campbell, P. K. E., & Middleton, E. M. (2021). Unraveling the  
 1010 physical and physiological basis for the solar- induced chlorophyll fluorescence and  
 1011 photosynthesis relationship using continuous leaf and canopy measurements of a corn  
 1012 crop. *Biogeosciences*, 18(2), 441–465. <https://doi.org/10.5194/bg-18-441-2021>
- 1013 Yang, P., Verhoef, W., & van der Tol, C. (2017). The mSCOPE model: A simple adaptation  
 1014 to the SCOPE model to describe reflectance, fluorescence and photosynthesis of  
 1015 vertically heterogeneous canopies. *Remote Sensing of Environment*, 201, 1–11.  
 1016 <https://doi.org/10.1016/j.rse.2017.08.029>
- 1017 Yin, T., Gastellu-Etchegorry, J.-P., Lauret, N., Grau, E., & Rubio, J. (2013). A new approach  
 1018 of direction discretization and oversampling for 3D anisotropic radiative transfer  
 1019 modeling. *Remote Sensing of Environment*, 135, 213–223.  
 1020 <https://doi.org/10.1016/j.rse.2013.03.030>
- 1021 Yin, T., Lauret, N., & Gastellu-Etchegorry, J.-P. (2015). Simulating images of passive sensors  
 1022 with finite field of view by coupling 3-D radiative transfer model and sensor  
 1023 perspective projection. *Remote Sensing of Environment*, 162, 169–185.  
 1024 <https://doi.org/10.1016/j.rse.2015.02.020>
- 1025 Yin, T., Lauret, N., & Gastellu-Etchegorry, J.-P. (2016). Simulation of satellite, airborne and  
 1026 terrestrial LiDAR with DART (II): ALS and TLS multi-pulse acquisitions, photon  
 1027 counting, and solar noise. *Remote Sensing of Environment*, 184, 454–468.  
 1028 <https://doi.org/10.1016/j.rse.2016.07.009>

## CHAPTER 4: IMPACT OF VEGETATION 3D STRUCTURE ON SIF

- 1029 Zeng, Y., Badgley, G., Chen, M., Li, J., Anderegg, L. D. L., Kornfeld, A., Liu, Q., Xu, B.,  
1030 Yang, B., Yan, K., & Berry, J. A. (2020). A radiative transfer model for solar induced  
1031 fluorescence using spectral invariants theory. *Remote Sensing of Environment*, 240,  
1032 111678. <https://doi.org/10.1016/j.rse.2020.111678>
- 1033 Zhang, Z., Zhang, Y., Porcar-Castell, A., Joiner, J., Guanter, L., Yang, X., Migliavacca, M.,  
1034 Ju, W., Sun, Z., Chen, S., Martini, D., Zhang, Q., Li, Z., Cleverly, J., Wang, H., &  
1035 Goulas, Y. (2020). Reduction of structural impacts and distinction of photosynthetic  
1036 pathways in a global estimation of GPP from space-borne solar-induced chlorophyll  
1037 fluorescence. *Remote Sensing of Environment*, 240, 111722.  
1038 <https://doi.org/10.1016/j.rse.2020.111722>
- 1039 Zhang, Z., Zhang, Y., Zhang, Q., Chen, J. M., Porcar-Castell, A., Guanter, L., Wu, Y., Zhang,  
1040 X., Wang, H., Ding, D., & Li, Z. (2020). Assessing bi-directional effects on the  
1041 diurnal cycle of measured solar-induced chlorophyll fluorescence in crop canopies.  
1042 *Agricultural and Forest Meteorology*, 295, 108147.  
1043 <https://doi.org/10.1016/j.agrformet.2020.108147>
- 1044 Zhao, F., Dai, X., Verhoef, W., Guo, Y., van der Tol, C., Li, Y., & Huang, Y. (2016).  
1045 FluorWPS: A Monte Carlo ray-tracing model to compute sun-induced chlorophyll  
1046 fluorescence of three-dimensional canopy. *Remote Sensing of Environment*, 187, 385–  
1047 399. <https://doi.org/10.1016/j.rse.2016.10.036>
- 1048 Zhao, F., Li, Y., Dai, X., Verhoef, W., Guo, Y., Shang, H., Gu, X., Huang, Y., Yu, T., &  
1049 Huang, J. (2015). Simulated impact of sensor field of view and distance on field  
1050 measurements of bidirectional reflectance factors for row crops. *Remote Sensing of*  
1051 *Environment*, 156, 129–142. <https://doi.org/10.1016/j.rse.2014.09.011>
- 1052

## 4.3 Conclusion

In this chapter, the impact of forest structure on SIF emission and observation was studied using realistic mock-ups derived from LiDAR. Results showed that neglecting the forest structure can lead to an overestimation of SIF radiance by up to 50% notably for oblique sun directions. The impact of vegetation structure was higher on the propagation of SIF within the canopy than on the PAR absorption and SIF emission. Results also showed that SIF radiance is overestimated if woody elements are neglected. This overestimation is more due to the shadowing effect than to the blocking effects of the woody elements. As already mentioned, this study was conducted after conversion of turbid voxels to quasi turbid medium because at that time, the turbid medium was not implemented yet in DART-Lux. The comparison of the turbid and the quasi-turbid representation showed that the turbid has a longer computation time but a lower Monte Carlo noise for the same number of samples. Should the work be redone, the quasi-turbid representation of vegetation would probably be used again.





# Chapter 5

## **Thermal emission and radiative budget modeling in DART-Lux**

Photosynthetically active vegetation continuously exchanges matter and energy with its environment via biochemical reactions and heat transfer processes. Energy exchanges can be separated into non-radiative (*e.g.*, sensible and latent heat exchanges) and radiative exchanges that consist in receiving energy through the absorption of incident radiation from the sun directly or after being scattered by the atmosphere and through the radiation emitted by the atmosphere and all the surrounding materials such as soil, woody elements, etc. and lose energy by emitting thermal radiation. The net absorbed radiation is therefore the difference between absorbed and emitted energy. Radiative energy exchanges are an important component of the energy balance of vegetation. Therefore, modeling the radiation budget including thermal emission is essential. The first section of this chapter presents the modeling of thermal emission and the second section presents the modeling of the radiative budget in DART-Lux.

## 5.1 Thermal emission modeling

### 5.1.1 Theoretical background

Thermal emission is an energy emission in the form of electromagnetic radiation from any material having a temperature  $T$  higher than the absolute zero (*i.e.*,  $T > 0$  K) due to the movement of molecules and atoms in the material.

The Planck law gives the spectral distribution of isotropic radiance emitted by a blackbody (*i.e.*, an ideal body that absorbs all the incident electromagnetic radiation) at temperature  $T$  (K):

$$L_B(\lambda, T) = \frac{2 \cdot h \cdot c^2}{\lambda^5} \cdot \frac{1}{e^{\frac{hc}{\lambda k T}} - 1} \quad (W \cdot m^{-2} \cdot m^{-1} \cdot sr^{-1}) \quad (5.1)$$

where  $\lambda$  is the wavelength in  $m$ ,  $h = 6.626\,070\,15 \times 10^{-34}$  J.s is the Planck's constant,  $c = 2.997\,924\,58 \times 10^8$   $m \cdot s^{-1}$  (in vacuum) is the speed of light, and  $k = 1,380\,649 \times 10^{-23}$  J.K<sup>-1</sup> is the Boltzmann constant.

The exitance of a Blackbody over the whole spectrum results from the integration of the Planck's law over the whole spectrum, and over the hemisphere ( $\times \pi$  for an isotropic radiance). It is given by the Stefan-Boltzmann law:

$$\begin{aligned} M_B(T) &= \pi \cdot \int_0^{+\infty} \frac{2 \cdot h \cdot c^2}{\lambda^5} \cdot \frac{1}{e^{\frac{hc}{\lambda k T}} - 1} d\lambda \\ &= \sigma \cdot T^4 \quad (W \cdot m^{-2}) \end{aligned} \quad (5.2)$$

where  $\sigma = \frac{2 \cdot \pi^5 \cdot k^4}{15 \cdot h^3 \cdot c^2} \approx 5.670374419 \times 10^{-8}$   $W \cdot m^{-2} \cdot K^{-4}$

Real bodies are not perfect emitters, the emitted radiance is scaled by their spectral emissivity:

$$L(\lambda, T) = \varepsilon(\lambda) \cdot L_B(\lambda, T) \quad (5.3)$$

For a spectral band  $(\lambda, \Delta\lambda)$ , the emitted radiance is computed as the average of the emitted radiance over this band:

$$L_{\lambda, \Delta\lambda}(T) = \frac{1}{\Delta\lambda} \int_{\lambda - \frac{\Delta\lambda}{2}}^{\lambda + \frac{\Delta\lambda}{2}} \varepsilon(\lambda) \cdot L_B(\lambda, T) d\lambda = \frac{\varepsilon_{\Delta\lambda}}{\Delta\lambda} \int_{\lambda - \frac{\Delta\lambda}{2}}^{\lambda + \frac{\Delta\lambda}{2}} L_B(\lambda, T) d\lambda \quad (5.4)$$

where  $\varepsilon_{\Delta\lambda}$  is the emissivity over the band  $(\lambda, \Delta\lambda)$ .

The brightness temperature  $T_B$  of an observed emitting body having a thermodynamic temperature  $T$  and an emissivity  $\varepsilon(\lambda)$  is the thermodynamic temperature a black body should have in order to have the radiance  $L(\lambda, T)$  of the emitting body at the wavelength  $\lambda$ . It is computed using the inverse function of the Planck law:

$$T_B(\lambda) = L_B^{-1}(L(\lambda, T), \lambda) = \frac{h \cdot c}{k \cdot \lambda \cdot \ln \left( 1 + \frac{2 \cdot h \cdot c^2}{\lambda^5 \cdot \varepsilon(\lambda) \cdot L_B(\lambda, T)} \right)} \quad (5.5)$$

If the emitting body is a blackbody, its brightness temperature is equal to its thermodynamic temperature for every wavelength. Otherwise, it is less than or equal to its thermodynamic temperature and is wavelength dependent.

For a spectral band  $(\lambda, \Delta\lambda)$ , instead of a single wavelength, the brightness temperature is:

$$T_B(\lambda, \Delta\lambda) = L_B^{-1}(L_{\lambda, \Delta\lambda}(T), \lambda_{eq}) \quad (5.6)$$

with  $\lambda_{eq}$  the wavelength between  $\lambda - \frac{\Delta\lambda}{2}$  and  $\lambda + \frac{\Delta\lambda}{2}$  for which the Planck function is equal to the average of the Planck function on the spectral band  $(\lambda, \Delta\lambda)$  for the temperature  $T$ . According to the mean value theorem,  $\lambda_{eq}$  exists. It is defined as:

$$L_B(\lambda_{eq}, T) = \frac{1}{\Delta\lambda} \cdot \int_{\lambda - \frac{\Delta\lambda}{2}}^{\lambda + \frac{\Delta\lambda}{2}} L_B(\lambda, T) d\lambda \quad (5.7)$$

### 5.1.2 Thermal emission for facets

From the point of view of the modelling of radiative transfer, the thermal emission of facets corresponds to the consideration of the emitting facets as light sources. This functionality is already implemented in the LuxCoreRender software. However, it is limited to single face emitters, and to constant radiance per object.

In a first step, the single face emitting facet has been adapted to create a double face emitting facet. This is done by sampling the whole sphere instead of the upper hemisphere when sampling an emission direction, and by making the material emit when it is hit by a ray from the upper or the lower side.

In a second step, other methods have been introduced in order to simulate more realistic temperature distributions than constant temperature per object.

**Simulation and importation of 3D temperature distribution**

*a) Illumination*

The illumination method is used in DART-FT to simulate a more or less realistic 3D temperature distribution based on the illumination of surfaces. The idea is that the most illuminated surfaces tend to have higher temperature and vice versa. This is an approximation since the temperature of a surface depends on many other parameters such as its heat capacity and its heat exchanges through conduction and convection; its estimation requires the computation of the full energy balance. However, the illumination method is a first approximation. It requires to specify the range of temperature ( $T_{mean}, \Delta T$ ) per type of element (e.g., wall with specific orientation). The first order irradiance (i.e., direct sun and atmosphere radiation) is used to distribute the temperature: the most illuminated surfaces are assigned the maximal temperature, the least illuminated surfaces are assigned the least temperature and intermediately illuminated surfaces are assigned intermediate temperature values.

In DART-Lux, the illumination method differs from DART-FT: rays are not sent from the source (i.e., sun and atmosphere) but from so-called emitting points in the scene elements of which the temperature must be computed. Therefore, for facets, the illumination method starts with the determination of emitting points in the scene elements. This is done by computing the intersection of each facet with a 3D regular grid. Then, scene facets are virtually segmented into sub-polygons, and the centroid of each sub-polygon (Figure 5-1) is treated as an emitting point. Any triangle that does not intersect the grid because it is too small is assigned an emitting point that is the centroid of this triangle.

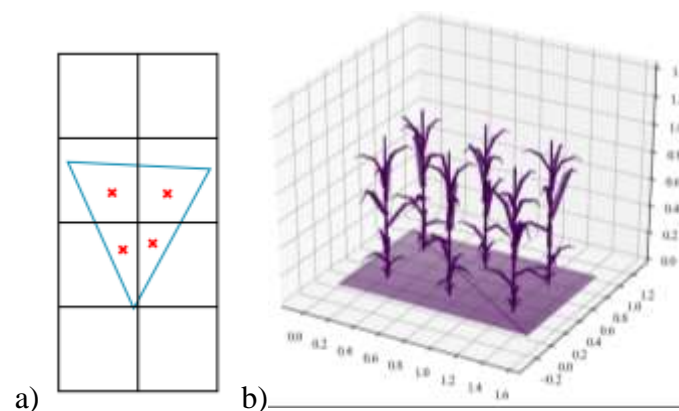


Figure 5-1: Points sampling method for a single triangle (a) and a maize scene (b)

Then, the irradiance (Figure 5-2) of the centroid of each facet, on the two sides of the facet, is computed using direct sun irradiance and atmosphere diffuse irradiance defined by a SKYL value. This order 1 irradiance  $E_{P,1}$  at each centroid  $P$  is:

$$E_{P,1} = E_{P,dir,1} + E_{P,diff,1} \quad (5.8)$$

With  $E_{P,dir,1}$  the direct order 1 irradiance computed by tracing a ray for the point  $P$  in the sun direction. If the ray is not intercepted,  $E_{P,dir,1} = E_{sun} \cdot |\Omega_s \cdot \vec{n}|$ , ( $E_{sun}$  is the sun irradiance for a surface perpendicular to the sun direction  $\Omega_s$  and  $\vec{n}$  is the surface normal, if  $\Omega_s \cdot \vec{n} > 0$ , the top face is illuminated, otherwise the bottom face is illuminated). If the ray is intercepted,  $E_{P,dir} = 0$ .

The incident diffuse radiation at a point  $P$  is:

$$E_{P,diff,1} = \int_{2\pi} L_{P,1}(\Omega_i) \cdot |\Omega_i \cdot \vec{n}| \cdot d\Omega \quad (5.9)$$

with  $L_{P,1}(\Omega_i)$  the order 1 diffuse radiance incident to the point  $P$ .

$E_{P,diff,1}$  is estimated using a Monte Carlo estimator  $\hat{E}_{P,diff,1}$  with  $N$  sampled directions  $\Omega_i$ :

$$\hat{E}_{P,diff,1} = \frac{1}{N} \cdot \sum_{i=1}^N \frac{L_{P,1}(\Omega_i) \cdot |\Omega_i \cdot \vec{n}|}{p(\Omega_i)} \quad (5.10)$$

The PDF for sampling a direction  $p(\Omega_i)$  verifies  $\int_{2\pi} p(\Omega_i) \cdot d\Omega = 1$ . The importance sampling is used. It requires that  $p(\Omega_i)$  has a similar shape to the integrand  $f(\Omega_i) = L_{P,1}(\Omega_i) \cdot |\Omega_i \cdot \vec{n}|$

Taking  $p(\Omega_i) = c \cdot |\Omega_i \cdot \vec{n}|$  with  $c \in \mathbb{R}$  (cosine distribution) leads to  $c = \frac{1}{\pi}$ , and Eq (5.10) becomes:

$$\hat{E}_{P,diff,1} = \frac{\pi}{N} \cdot \sum_{i=1}^N L_{P,1}(\Omega_i) \quad (5.11)$$

$\hat{E}_{P,diff,1}$  is unbiased. Its expected value is equal to the real value  $E_{P,diff,1}$  (cf. Appendix 5-1).

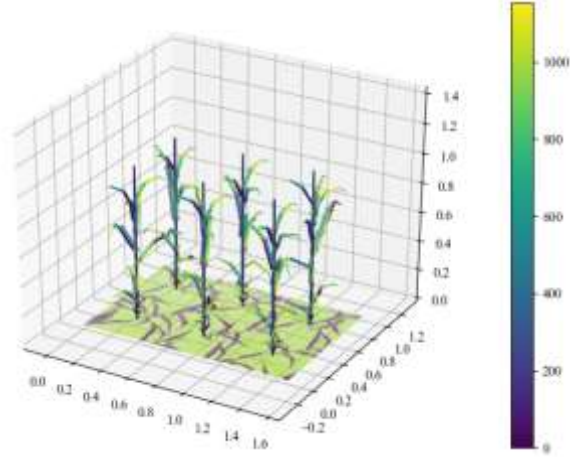


Figure 5-2: Local irradiance computed over the maize scene

Once the local irradiance is computed, a temperature  $T_P$  is assigned for each irradiance value  $E_P$  (Figure 5-3), using the user-defined temperature properties ( $T_{mean}, \Delta T$ ) and the relationship:

$$T_P^4 = a \cdot E_P + b \quad (5.12)$$

This relationship is chosen because for a surface at the thermal equilibrium with temperature  $T$  and receiving an energy flux  $E$ ,  $T^4$  increases linearly with  $E$ .

$a$  and  $b$  are compute such that  $T_{max}^4 = a \cdot E_{max} + b$  and  $T_{min}^4 = a \cdot E_{min} + b$ :

$$a = \frac{T_{max}^4 - T_{min}^4}{E_{max} - E_{min}} \quad (5.13)$$

$$b = T_{max}^4 - a \cdot E_{max} \quad (5.14)$$

Therefore:

$$T_P = \left( \frac{T_{max}^4 - T_{min}^4}{E_{max} - E_{min}} \cdot (E_P - E_{max}) + T_{max}^4 \right)^{\frac{1}{4}} \quad (5.15)$$

We note from Eq (5.15) that if  $E_{max}$ ,  $E_{min}$  and  $E_P$  are multiplied by a factor  $\alpha$ , the expression of  $T_P$  remains the same. Hence, the absolute value of BOA irradiance  $E_{BOA}$  used in the illumination step is not important. Therefore, any dummy value can be used and there is no need compute the real BOA irradiance or to perform a multispectral illumination.

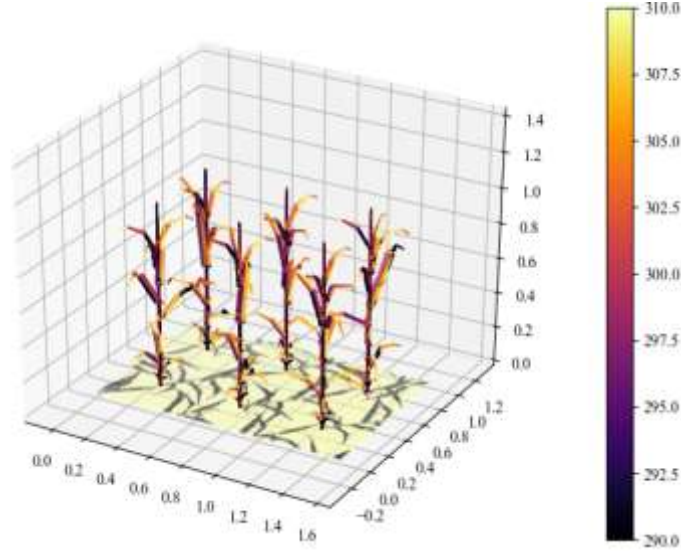


Figure 5-3: Temperature distribution computed over the maize scene

Once the temperature distribution is computed, the radiative transfer simulation starts.

*b) Sunlit and shaded temperatures*

For some applications including SIF emission, one need to know the thermodynamic temperature of sunlit ( $T_{su}$ ) and shaded ( $T_{sh}$ ) parts for each type of element of the scene, and to use them in a radiative transfer model. This possibility was introduced in DART-Lux based on the illumination method described in the previous section.

A sunlit fraction is computed at each point, as the ratio between the order 1 local irradiance, and the local irradiance the point would receive if it was totally sunlit:

$$f_{sunlit} = \frac{E_P}{\frac{E_{dir,BOA}}{\cos(\theta_s)} \cdot |\Omega_l \cdot \Omega_s| + E_{diff,BOA}} \quad (5.16)$$

The emitted radiance by this point is then:

$$L_{\lambda,\Delta\lambda}(T_{su}, T_{sh}, f_{sunlit}) = f_{sunlit} \cdot L_{\lambda,\Delta\lambda}(T_{su}) + (1 - f_{sunlit}) \cdot L_{\lambda,\Delta\lambda}(T_{sh}) \quad (5.17)$$

*c) Imported SCOPE temperature profiles*

Some 1D models that compute the full energy balance such as SCOPE provide 1D temperature profiles for sunlit and shaded leaves. The temperature profiles provided by SCOPE are function of the height within the canopy for shaded leaves  $T_{sh}(z)$  and the leaf zenith angle, azimuth angle and height within the canopy for sunlit leaves  $T_{su}(z, \theta_l, \varphi_l)$ . DART-Lux can import these



Some 1D models of canopy energy balance simulate 1D temperature profiles for leaves. The SCOPE model simulates a 1D temperature profile for sunlit leaves and another one for shaded leaves. The temperature profiles from SCOPE are function of the height in the canopy for shaded leaves  $T_{sh}(z)$  and on the leaf zenith angle, the azimuth angle and the height in the canopy for sunlit leaves  $T_{su}(z, \theta_l, \varphi_l)$ . DART-Lux was adapted to import these temperature profiles and to simulate radiative transfer with them. To this end, the sunlit fraction  $f_{sunlit}$  is computed using Eq (5.16) and the emitted radiance is computed using Eq (5.17), the temperatures  $T_{sh}$  and  $T_{su}$  being interpolated from the imported SCOPE temperature profiles according to the height of the centroid for  $T_{sh}$ , and according to the height of the centroid and the zenith and azimuth angles of the normal vector of the facet for  $T_{su}$ .

*d) Importation of 3D temperature distribution*

DART-Lux was adapted to import any 3D temperature distribution. The approach relies on a division of the scene into “voxels” at any 3D resolution and on the assignation of the corresponding temperature to all scene elements inside each voxel. 3D temperature distributions can be provided by other models like fire models (*e.g.*, Y. Liu et al. 2019). In addition, 2D temperature distributions, for example derived from the inversion of remote sensing images, can also be imported.

***Radiative transfer simulation***

Once the temperature distribution is computed and/or imported, the radiative transfer simulation starts. The temperature distribution methods provide discrete temperature values for points distributed over the scene or for virtual voxels. This is done only for the central scene and not for the eventual repeated scenes (*i.e.*, duplications of the scene of interest in order to simulate its neighborhood). However, in reality, any point in the scene can emit if sampled or intercepted by a ray, including points outside the central scene (*i.e.*, scene of interest). Therefore, to compute the emitted radiance of any point  $M$  in the scene, its corresponding point in the central scene  $M_c$  is computed first using a horizontal shift. If the temperature is defined using a temperature profile, the temperature of the voxel containing  $M_c$  is assigned to  $M$ . Otherwise, the nearest point to  $M_c$  with an assigned temperature is searched over the scene (Figure 5-3) and its temperature is assigned to  $M$ . The search operation is optimized using a Bounding Volume Hierarchy (BVH) structure implementation from LuxCoreRender.

### 5.1.3 Thermal emission for volumes

The modeling of thermal emission of volumes filled with homogeneous fluids or turbid medium has been designed and implemented into DART-Lux.

#### *Volumes with spatially constant temperature*

Let us consider a volume homogeneously filled with a fluid or turbid medium at constant thermodynamic temperature  $T$ , and a ray sent from the sensor (Figure 5-4) that enters the volume at a point  $A$ . Then, the order 1 thermal emission of the volume is computed.

For a volume filled with a fluid, the radiance emitted by an elementary layer of the volume of height  $dz$  and seen by the sensor is:

$$dL = \sigma_t \cdot dz \cdot L_{\lambda, \Delta\lambda}(T) \cdot e^{-\sigma_t \cdot z} \quad (5.18)$$

with  $\sigma_t \cdot dz$  the area of emitting particles in the layer  $dz$  per horizontal surface unit,  $L_{\lambda, \Delta\lambda}(T)$  the emitted particle radiance and  $e^{-\sigma_t \cdot z}$  the transmittance between the layer  $dz$  and point  $A$ .

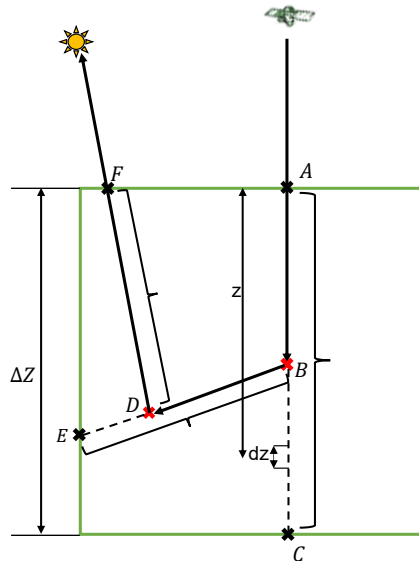


Figure 5-4: Schematic representation of the volume thermal emission

For a volume filled with turbid medium:

$$dL = G(\Omega_v) \cdot u_l \cdot dz \cdot L_{\lambda, \Delta\lambda}(T) \cdot e^{-G(\Omega_v) \cdot u_l \cdot z} \quad (5.19)$$

with  $G(\Omega_v) \cdot u_l \cdot dz$  the effective area of emitting leaves in the layer  $dz$  per horizontal surface unit,  $L_{\lambda, \Delta\lambda}(T)$  the emitted leaf radiance and  $e^{-G(\Omega_v) \cdot u_l \cdot z}$  the transmittance between the layer  $dz$  and point  $A$ .

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By integrating over the segment  $[AC]$  (*i.e.*, whole volume), we get the radiance  $L_{order1}$  emitted along this segment at order 1 and seen by the sensor. For a volume filled with a fluid, we get:

$$\begin{aligned} L_{order1} &= \int_{\Delta Z} dL = \int_0^{\Delta Z} \sigma_t \cdot L_{\lambda, \Delta \lambda}(T) \cdot e^{-\sigma_t \cdot z} \cdot dz \\ &= L_{\lambda, \Delta \lambda}(T) \cdot (1 - e^{-\sigma_t \cdot \Delta Z}) \end{aligned} \quad (5.20)$$

Similarly, for a volume filled with turbid medium:

$$L_{order1} = L_{\lambda, \Delta \lambda}(T) \cdot (1 - e^{-G(\Omega_v) \cdot u_t \cdot \Delta Z}) \quad (5.21)$$

Multiple order emission is simulated as successive order 1 emission whenever the ray sent from the sensor is intercepted at a point  $B$ . Then, a scattering direction  $\overline{BE}$  is sampled, with  $E$  being the interception of the scattering direction and the edge of the volume. The emission along the segment  $[BE]$  seen at  $B$  is computed using Eq (5.20) or (5.21) and scattered at  $B$  towards the sensor. Then, a travel distance is sampled over  $\overline{BE}$ . If the sampling leads to an interception in point  $D$  within the volume, a new scattering direction  $\overline{DF}$  is sampled, and the emission along  $[DF]$  seen at  $D$  is computed and scattered towards  $B$ , and so on until a sampled travel distance is outside the volume, or until the specified maximal scattering order is reached.

***Illumination method and sunlit fraction for volumes***

For a horizontally infinite homogeneous turbid medium, as for SCOPE, the sunlit and shaded fractions of leaves are computed statistically using the Beer law. For a layer at height  $z$  inside a canopy of height  $\Delta Z$ , we have:

$$f_{sunlit}^{layer}(z) = e^{-G(\Omega_s) \cdot u_l \cdot \frac{\Delta Z - z}{\cos \theta_s}} = \frac{E_{dir}(z)}{E_{dir, BOA}} \quad (5.22)$$

This definition is extended to compute the average fraction of sunlit leaves in a turbid cell:

$$\bar{f}_{sunlit}^{cell} = \frac{1}{E_{BOA} \cdot \Delta Z} \int_0^{\Delta Z} E(z) \cdot dz \quad (5.23)$$

The computation of the integral in Eq (5.23) would require to divide the cell into smaller layers and to compute the irradiance at each layer, which would be very computationally expensive.

Instead, an approximation is made by assuming that the cell is inside an infinite homogeneous layer of the same height as the cell. Then,  $\bar{f}_{sunlit}^{cell}$  becomes:

$$\bar{f}_{sunlit}^{cell} \approx \frac{1}{\Delta Z} \int_0^{\Delta Z} e^{-G(\Omega_s) \cdot u_l \cdot \frac{\Delta Z - z}{\cos \theta_s}} dz \quad (5.24)$$

According to the mean value theorem, there exists a height  $z_{eq}$  such that:

$$e^{-G(\Omega_s) \cdot u_l \cdot \frac{\Delta Z - z_{eq}}{\cos \theta_s}} = \frac{1}{\Delta Z} \int_0^{\Delta Z} e^{-G(\Omega_s) \cdot u_l \cdot \frac{\Delta Z - z}{\cos \theta_s}} dz \quad (5.25)$$

Thus, the irradiance at the height  $z_{eq}$  is approximately equal to the mean irradiance over the cell, and therefore:

$$\bar{f}_{sunlit} \approx \frac{E(z_{eq})}{E_{BOA}} \quad (5.26)$$

$E(z_{eq})$  is also used for assigning a temperature to the cell.

### ***Volumes with spatially variable temperatures***

The illumination method for temperature distribution for volumes gives a 3D temperature array. A 3D temperature array can also be imported directly. However, a volume is not necessarily contained by a single cell. The same volume can then have different temperatures if it is contained in more than one cell. DART-Lux has been adapted to manage these volumes.

Let us consider a homogenous cell filled with turbid medium, of height  $H$ . It is divided into 2 layers, the bottom layer of height  $h$  has a temperature  $T_1$  and the top layer of height  $H - h$  has a temperature  $T_2$ . For a ray coming from the sensor from at the nadir direction for example, entering the volume, a distance is randomly sampled inside the volume. The PDF  $p(l)$  for sampling this distance is proportional to the Beer law and verifies the following normalization equality:

$$\int_0^H p(l) \cdot dl = 1 \quad (5.27)$$

Therefore (c.f. Appendix 5-2),

$$p(l) = \frac{G(\Omega) \cdot u_l \cdot e^{-G(\Omega) \cdot u_l \cdot l}}{1 - e^{-G(\Omega) \cdot u_l \cdot H}} \quad (5.28)$$

By sampling a distance  $l$  according to this PDF, the obtained distance is between 0 and  $H$ . If  $l < H - h$ , the observed radiance is computed assuming that the volume has a constant temperature  $T_2$ , otherwise, the observed radiance is computed assuming that the volume has a constant temperature  $T_1$ . In Appendix 5-2, we show that the expected value of order 1 radiance computed using this sampling technique is equal to the true value of observed order 1 radiance. Since the multiple order emission is treated as successive order 1 emissions, this method allows one to simulate thermal emission observations for homogeneous volumes.

#### 5.1.4 Results

Six scene examples are shown below to assess the accuracy of the developed modeling and to illustrate some potential uses:

##### *Synthetic scene (Facets)*

The thermal emission modeling and the temperature determination method using illumination are first assessed by comparison with DART-FT. Figure 5-5 shows the brightness temperatures images simulated using DART-FT (CT = 5 min 45 s, RAM = 1.9 GB) and DART-Lux (CT = 24 s, RAM = 1.2 GB) for the same synthetic scene made of facets only with three trees and a house whose roof has four parts. The average image radiance is  $14.134 \text{ W} \cdot \text{m}^{-2} \cdot \mu\text{m}^{-1} \cdot \text{sr}^{-1}$  for DART-FT and  $14.119 \text{ W} \cdot \text{m}^{-2} \cdot \mu\text{m}^{-1} \cdot \text{sr}^{-1}$  for DART-Lux. The DART-FT image has many pixels with extreme values at the level of the trees caused by discretization effects. The scene is  $20 \times 20 \text{ m}^2$  and the spatial resolution is 5 cm. The temperature distribution is determined using the illumination method with direct illumination only. In both DART-FT and DART-Lux images, we note that sunlit ground has a higher temperature than shaded ground. Also, the four parts of the roof give four different signals because they receive different direct illumination, depending on their orientation relatively to the solar direction.

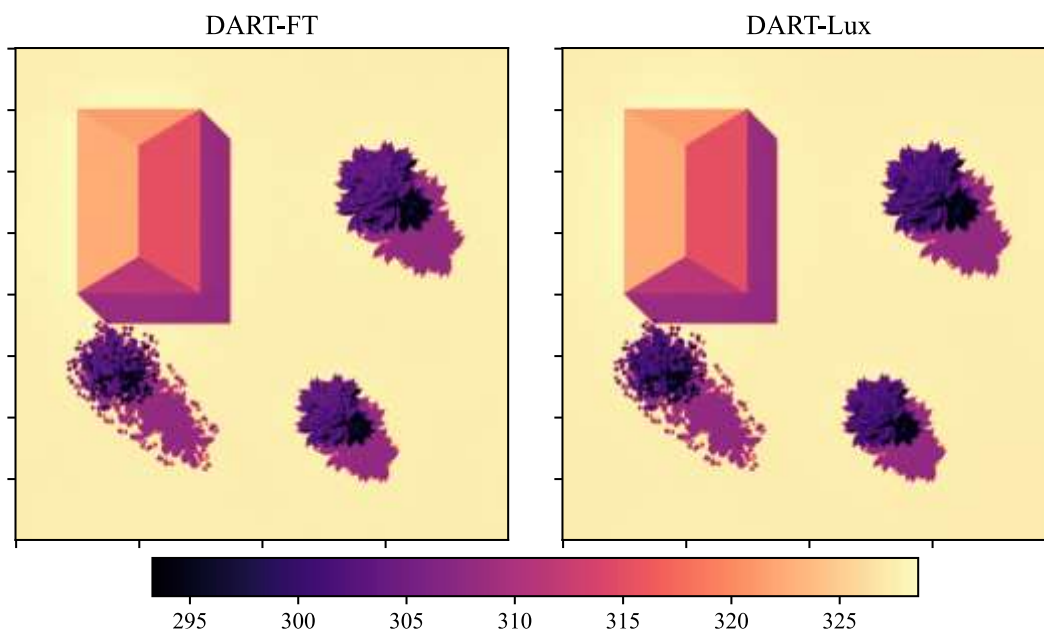


Figure 5-5: Nadir brightness temperature (K) images simulated by DART-FT and DART-Lux for a simple synthetic scene at 10  $\mu\text{m}$ .

### *Turbid volume*

Thermal emission modeling in volumes is assessed by comparison with DART-FT for a simple turbid volume on top on a non-emitting and a non-reflective ground. The turbid volume has a LAI = 1, a spherical LAD, a thermodynamic temperature equal to 290 K, and leaf reflectance and transmittance both equal to 0.06 (*i.e.*, 0.88 emissivity). Figure 5-6 shows the comparison of simulated radiance between DART-FT (CT = 1 min 2 s) and DART-Lux (CT = 8 s) between 8 and 14  $\mu\text{m}$ .

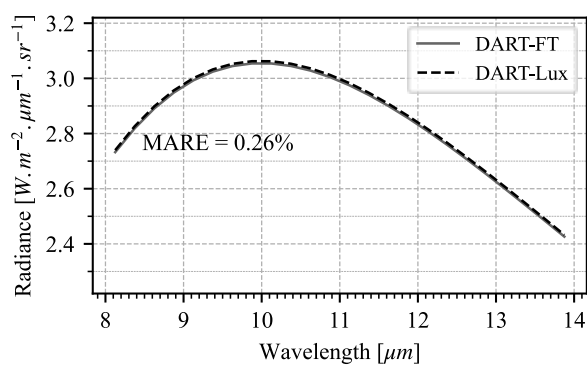


Figure 5-6: Radiance comparison between DART-FT and DART-Lux for a simple turbid plot

**Realistic urban scene: Brienne district (Toulouse)**

Figure 5-7 shows a brightness temperature image of the Brienne district in Toulouse, simulated using DART-FT (CT = 1 h 30 min, RAM = 23.25 GB) and DART-Lux (8 min 32 s, RAM = 33.58 GB) at 10  $\mu\text{m}$  wavelength. The scene is  $750 \times 1400 \text{ m}^2$  and the spatial resolution is 1 m. The temperature distribution is computed illumination (direct only) with a mesh grid resolution of 0.5 m in DART-Lux and an illumination step of 0.5 in DART-FT. The average image radiance is  $10.340 \text{ W} \cdot \text{m}^{-2} \cdot \mu\text{m}^{-1} \cdot \text{sr}^{-1}$  for DART-FT and  $10.360 \text{ W} \cdot \text{m}^{-2} \cdot \mu\text{m}^{-1} \cdot \text{sr}^{-1}$  for DART-Lux. Extreme values pixel are observed in the DART-FT image. For a more accurate DART-FT simulation, more discretization parameters are required which would increase computation time and memory requirements.

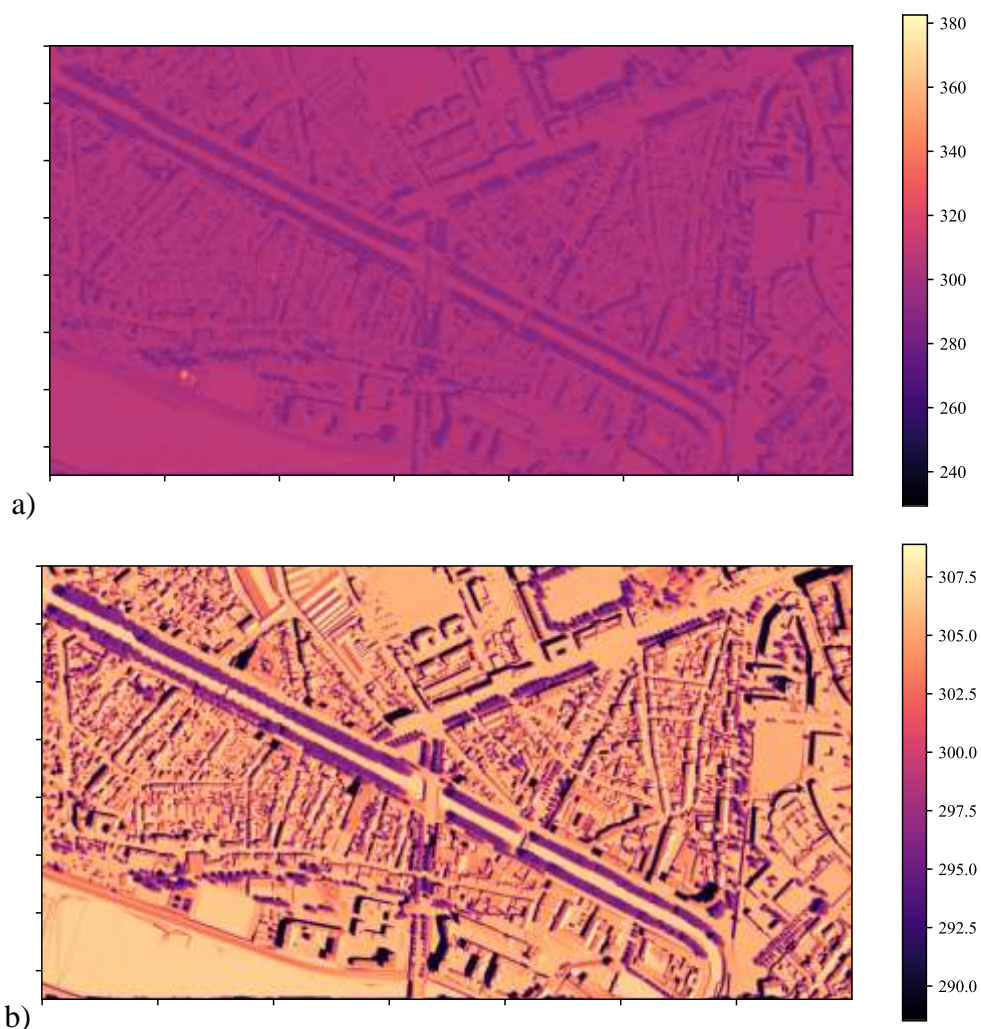


Figure 5-7: Nadir brightness temperature (K) images at 10  $\mu\text{m}$  of the Brienne district, Toulouse ( $750 \times 1400 \text{ m}^2$ , 1 m resolution) simulated by DART-FT (a) and DART-Lux (b)

***Realistic forest scene: SERC forest***

Figure 5-8 shows an airborne brightness temperature image taken by the NASA's GLiHT thermal infrared imager (spectral range [8 – 14  $\mu\text{m}$ ]) over the SERC forest (Maryland, USA), and its corresponding image simulated with DART-Lux. The mock-up is a 3D distribution of voxels derived from the GLiHT airborne LiDAR measurements. It is  $600 \times 600 \text{ m}^2$  large with 0.5 m voxel dimension. In the absence of a measurements of 3D temperature distribution, the temperature was distributed using the illumination with a priori minimal and maximal temperature values for vegetation and ground, and a priori emissivities. To mimic the airborne image, the modeling of a pushbroom camera was introduced into DART-Lux. It was used to simulate this image. Although only approximate input parameters were used, the simulated images shows some visual similarities with the real image. This simulation cannot be run with DART-FT due to large computational requirements.

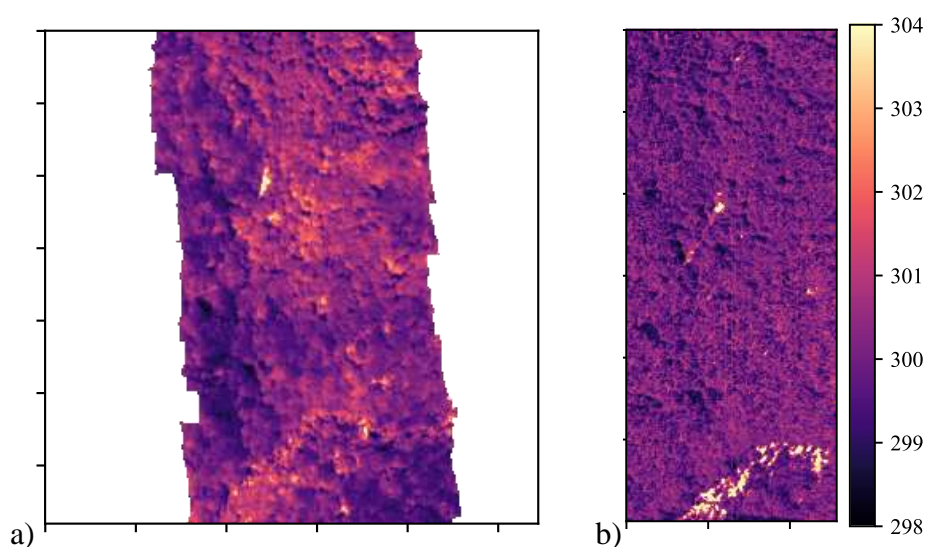


Figure 5-8: Brightness temperature (K) image (8 – 14  $\mu\text{m}$ ) over the SERC forest a) GLiHT image b) DART-Lux simulated image

***Realistic maize field***

Figure 5-9 shows images of a maize field in Auzeville, France, used in the frame of the calibration of the future TRISHNA satellite mission. They were acquired using a thermal camera (7.7 – 13  $\mu\text{m}$ ) at different positions. Figure 5-9 also shows the corresponding DART-Lux images. In these simulations, the mock-up was constructed respecting the real field



geometry and a single 3D maize plant object assumed to be representative. No LAI calibration was done. Leaves emissivity were measured from sample leaves from the field and temperature was distributed using the illumination method, with a priori temperature values because no temperature measurements were performed on the leaves. This is not a fully relevant comparison with field measurements, however, visual similarities with the simulated images can be observed.

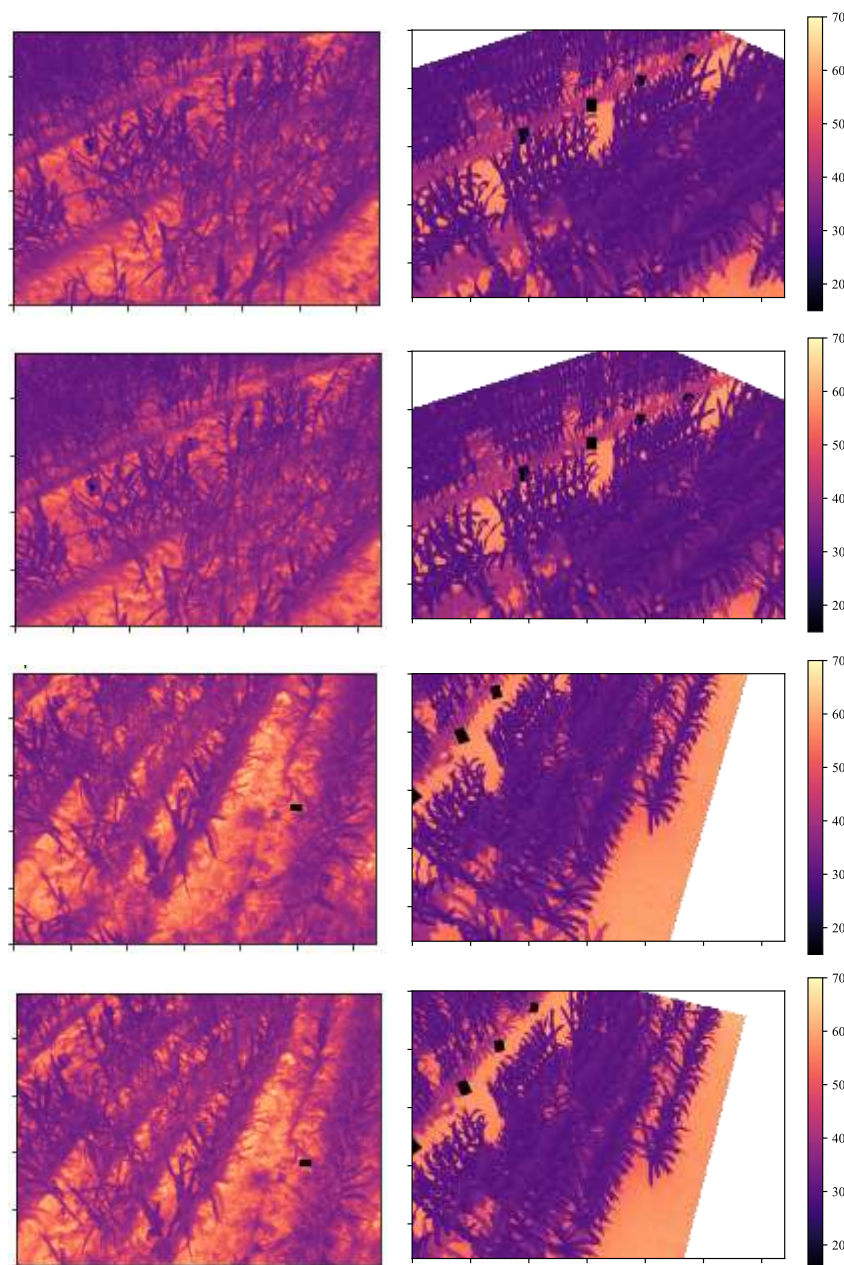


Figure 5-9: Thermal camera images (7.7 – 13  $\mu\text{m}$ ) of a maize field (left) and corresponding DART-Lux simulations ( $^{\circ}\text{C}$ )

**Fire simulation**

DART-Lux is also able to simulate fire simulation using volumes filled with fluids. As an example of fire application to DART-lux, we simulated an open vegetation fire scene, generated using the physical fire model FDS (McGrattan et al., 2013), which is part of the set of validation simulation of FDS (Case 064). It is based on measurements of a 1-ha experimental homogeneous grassland fire conducted in Australia (Mell et al., 2007). The scene is simulated using the latest FDS version to date (FDS6) and provides at 25 cm spatial resolution for several time steps 3D distribution of temperature, gas molar fraction for CO<sub>2</sub>, CO, H<sub>2</sub>O and soot volume fraction. The scene is input to DART using the DAO tool to load fluids as voxels and the temperature is included using a 3D temperature file created from the FDS output scene.

The simulated fire image is for a Middle Infra-Red (MIR) camera, the agema 550, which has a narrow spectral band located at 3.9  $\mu\text{m}$ . This spectral band is often used in fire monitoring. Figure 5-10 show nadir image simulated by DART-Lux, 50s after the ignition of the fire. During the experiment, only visible images were collected, so no image-to-image comparison is possible. Flames show brightness temperatures in an expected range in field scale propagating fire (>600K (Paugam et al., 2013)).

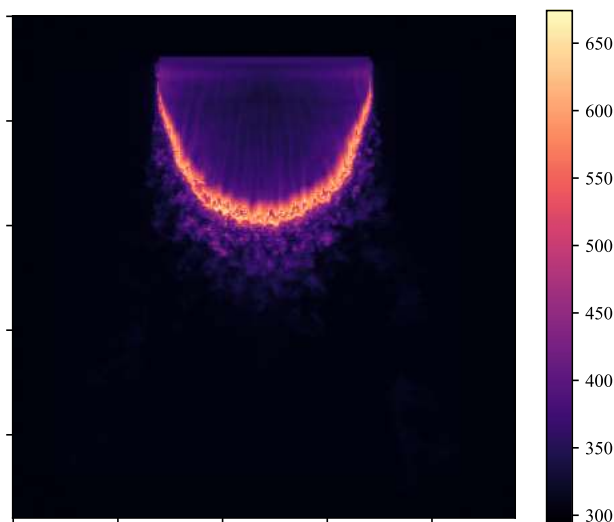


Figure 5-10: Nadir brightness temperature (K) image of a fire over a vegetated scene. (Courtesy of Ronan Paugam)

## 5.2 Radiative budget modeling in DART-Lux

DART-Lux uses the bi-directional path tracing algorithm to estimate sensor-level radiance using Monte Carlo integration techniques. It only computes end-to-end (*i.e.*, light source to sensor) radiance contribution of sampled light paths. Hence, this method does not provide information about the amount and the fate of radiation (*i.e.*, interception, scattering, absorption) at each vertex of these light paths. Therefore, unlike DART-FT, the simulation of images by DART-Lux is not adapted to the simultaneous simulation of the radiative budget.

An alternative method was developed to overcome this limitation. It takes advantage of the efficient bi-directional radiance computation method of DART-Lux to have an estimation of the local radiative budget at a number of points distributed over the scene. Then, all the different radiative budget products (per facet, per voxel) are derived: 3D radiative budget per type of scene element, including vertical profiles and total radiative budget per type of scene element. These radiative budget products are well adapted to the simulation of photosynthesis of 3D plants. For example, they provide information on the radiation that is absorbed chlorophylls. This method is developed for scene elements simulated as facets and as volumes.

### 5.2.1 Scene elements simulated as facets

Eq (5.11) introduced in the illumination method for distributing temperature in the scene presented in Section 0 is used to estimate the local order 1 irradiance for a point  $P$  of the scene. This equation can be extended to compute the row vector spectral irradiance  $\hat{E}_{\lambda,P,n}$  of order  $n$ :

$$\hat{E}_{\lambda,P,n} = \frac{\pi}{N} \cdot \sum_{i=1}^N L_{\lambda,P,n}(\Omega_i) \quad (5.29)$$

with  $L_{\lambda,P,n}(\Omega_i)$  the row vector of order  $n$  spectral radiance incident to the point  $P$ .

Having estimated the local incident spectral radiation, the scattered  $E_{\lambda,P,scat}$  and absorbed  $E_{\lambda,P,abs}$  spectral radiation vectors can be deduced:

$$\hat{E}_{\lambda,P,scat} = \begin{cases} \hat{E}_{\lambda,P,n} * \rho_{\lambda} \text{ (backward scattering)} \\ \hat{E}_{\lambda,P,n} * \tau_{\lambda} \text{ (forward scattering)} \end{cases} \quad (5.30)$$

$$\hat{E}_{\lambda,P,abs} = \hat{E}_{\lambda,P,scat} * (1 - \omega_{\lambda}) \quad (5.31)$$

with  $\rho_\lambda$  and  $\tau_\lambda$  the hemispherical spectral reflectance and transmittance vectors respectively at the point  $P$  and the spectral band  $(\lambda, \Delta\lambda)$ , and  $\omega_\lambda = \rho_\lambda + \tau_\lambda$  the single scattering albedo,  $(*)$  is the vector element-wise product operator.

In presence of SIF emission, it is also deduced as the product of the vector of spectral irradiance by the corresponding excitation emission fluorescence matrix:

$$\hat{E}_{\lambda,P,SIF} = \begin{cases} \hat{E}_{\lambda,P,n} \times M_{PSx,backward} & \text{(backward SIF)} \\ \hat{E}_{\lambda,P,n} \times M_{PSx,forward} & \text{(forward SIF)} \end{cases} \quad (5.32)$$

with  $(\times)$  the ordinary matrix product operator.

The thermally emitted radiation is computed directly from the local temperature  $T$ :

$$E_{\lambda,P,emis} = \pi \cdot L_{\lambda,\Delta\lambda}(T) \quad (5.33)$$

### 5.2.2 Scene elements simulated as volumes

The bi-directional Monte Carlo rendering method previously presented for volumes allows one to simulate images of scenes containing these volumes. It allows one to sample light paths and to evaluate the contribution of these paths to the radiance observed by the sensor. It does not provide information about the intercepted, scattered, absorbed radiation along these paths. A method to compute these quantities for volumes was developed.

A volume acquires radiative energy from ingoing radiation from its boundaries  $E_{V,in}$  and from emission  $E_{V,emis}$ , and loses the radiative energy that exits through its boundaries  $E_{V,out}$  and by absorption  $E_{V,abs}$ . The energy conservation principle states:

$$E_{V,in} + E_{V,emis} = E_{V,out} + E_{V,abs} \quad (5.34)$$

The method used for computing facets radiative budget can also be used to compute the incident radiation of the two sides of the boundary surfaces of volumes and therefore it allows to compute the estimations of the spectral ingoing  $\hat{E}_{\lambda,V,in}$  and outgoing  $\hat{E}_{\lambda,V,out}$  radiation vectors.

In presence of thermal emission, the spectral emission  $E_{\lambda,V,emis}$  can be computed knowing the spectral emitted radiance  $L_{\lambda,\Delta\lambda}$  and the total area of leaves  $A_l$  inside the volume for turbid volumes. For each spectral band  $(\lambda, \Delta\lambda)$ :

$$E_{\lambda,V,emis} = 2 \cdot \pi \cdot A_l \cdot L_{\lambda,\Delta\lambda} \quad (5.35)$$

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IN DART-LUX*

For a fluid volume of total volume  $V$ :

$$E_{\lambda,V,emis} = 4. \pi. V. \sigma_{t,\Delta\lambda} * L_{\Delta\lambda} \quad (5.36)$$

Therefore, the absorbed radiation can be estimated, and consequently the estimations of intercepted radiation  $\hat{E}_{\lambda,V,int}$  and the scattered radiation  $\hat{E}_{\lambda,V,scat}$  can be deduced knowing the spectral single scattering albedo  $\omega_\lambda$ .

$$\hat{E}_{\lambda,V,abs} = \hat{E}_{\lambda,V,in} - \hat{E}_{\lambda,V,out} + E_{\lambda,V,emis} \quad (5.37)$$

$$\hat{E}_{\lambda,V,int} = \frac{\hat{E}_{\lambda,V,abs}}{1 - \omega_\lambda} \quad (5.38)$$

$$\hat{E}_{\lambda,V,scat} = \hat{E}_{\lambda,V,int} \times \omega_\lambda \quad (5.39)$$

Where  $\div$  is the vector element-wise division operator.

We note from Eq (5.38) that if for a given spectral band  $(\lambda_i, \Delta\lambda_i)$ ,  $E_{\lambda_i,V,abs} = 0$ , and therefore  $\omega_{\lambda_i} = 1$ , it is impossible to compute  $\hat{E}_{\lambda_i,V,int}$  and therefore  $\hat{E}_{\lambda_i,V,scat}$ . In case  $\omega_{\lambda_i}$  is close to 1,  $E_{\lambda_i,V,abs}$  is small compared to  $E_{\lambda_i,V,in}$  and  $E_{\lambda_i,V,out}$  and this causes high variance of  $\hat{E}_{\lambda_i,V,abs}$ ,  $\hat{E}_{\lambda_i,V,int}$  and  $\hat{E}_{\lambda_i,V,scat}$  (c.f. Appendix 5-3).

In presence of SIF emission, the spectral emission  $E_{emis}$  can be estimated using the fluorescence excitation emission matrix  $M_{PSx} = M_{PSx,backward} + M_{PSx,forward}$ :

$$\hat{E}_{\lambda,V,emis} = \hat{E}_{\lambda,V,int} \times M_{PSx} \quad (5.40)$$

Therefore, Eq (5.34) gives:

$$\hat{E}_{\lambda,V,in} - \hat{E}_{\lambda,V,out} = \hat{E}_{\lambda,V,int} * (1 - \omega_\lambda) + \hat{E}_{\lambda,V,int} \times M_{PSx} \quad (5.41)$$

And consequently

$$\hat{E}_{\lambda,V,int} = (\hat{E}_{\lambda,V,in} - \hat{E}_{\lambda,V,out}) \times (I - diag(\omega_\lambda) - M_{PSx})^{-1} \quad (5.42)$$

Where  $I$  is the identity matrix and  $(.)^{-1}$  is the matrix inversion operator.

### 5.2.3 Results

#### *Scene elements simulated as facets*

Figure 5-11 shows a radiative budget product (intercepted radiation per facet) of a maize field computed using DART-Lux and compared DART-FT. The results provided by the two modes are similar. However, computation time is longer for DART-Lux (1 min 39 s) compared to DART-FT (54 s). From, the intercepted radiation, the scattered and absorbed radiation as well as the SIF emission (only for SIF emission bands) can be derived (Figure 5-14). The emitted thermal radiation is computed independently and directly from the local temperature (Figure 5-14).

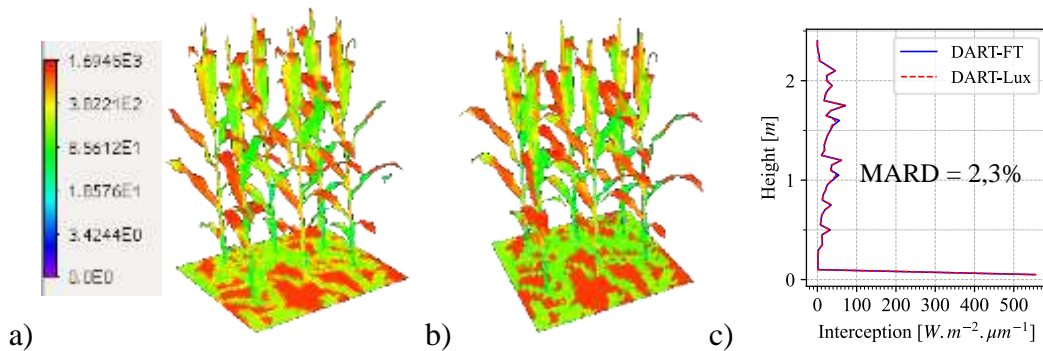


Figure 5-11: Intercepted radiation ( $W.m^{-2}.\mu m^{-2}$ ) for a visible band in of a maize field computed using a) DART-FT b) DART-Lux c) vertical profile comparison

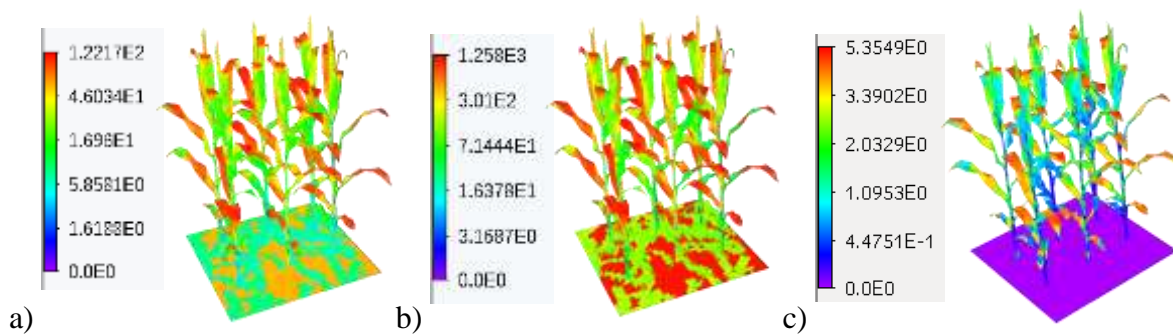


Figure 5-12: a) Scattered radiation, b) absorbed radiation and c) SIF emission ( $W.m^{-2}.\mu m^{-2}$ ) per facet computed by DART-Lux.

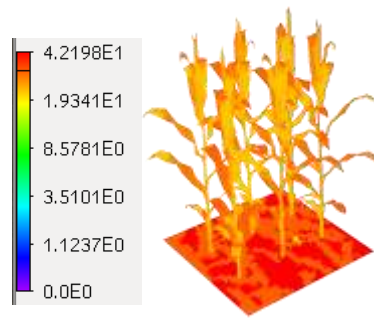


Figure 5-13: Emitted thermal radiation ( $\text{W}\cdot\text{m}^{-2}\cdot\mu\text{m}^{-2}$ ) computed by DART-Lux

*Scene elements simulated as turbid*

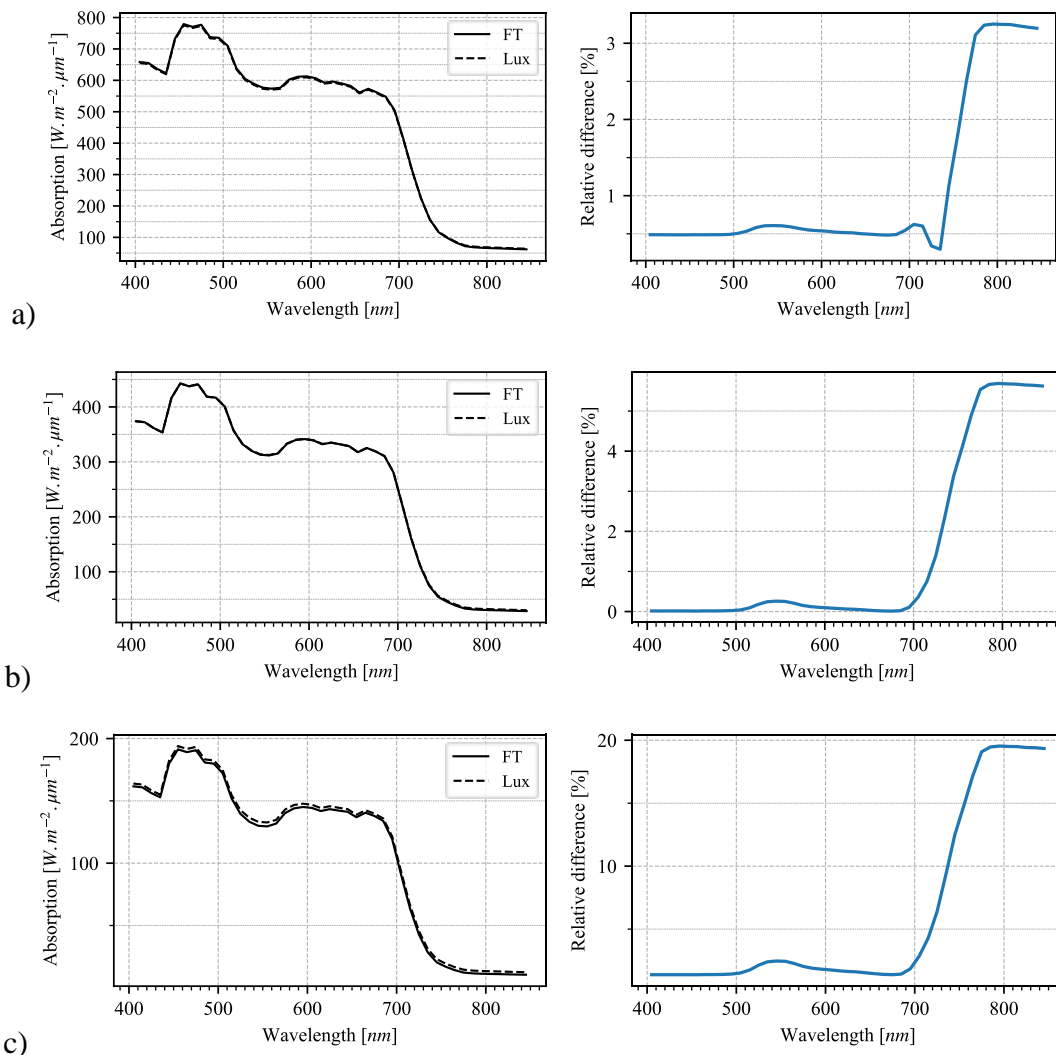


Figure 5-14: Absorbed radiation of a turbid plot computed by DART-Lux compared to DART-FT a) LAI = 1, b) LAI = 0.5, c) LAI = 0.2

## 5.2 RADIATIVE BUDGET MODELING IN DART-LUX

Figure 5-14 shows a radiative budget product (absorbed radiation) of a turbid plot computed by DART-Lux and compared to DART-FT for different LAI values. As mentioned in Section 2255.2.2, the estimation of absorbed radiation is less accurate (*i.e.*, higher relative difference with DART-FT considered here as reference) for high values of single scattering albedo, *i.e.*, for near infrared bands. Moreover, the smaller the LAI value is, the smaller is the absorption and the less accurate is its estimation by DART-Lux.

Although the absorption estimation is not accurate in the near infrared, we can get a good estimation of the emitted SIF as shown because it is only due to absorption in the visible domain

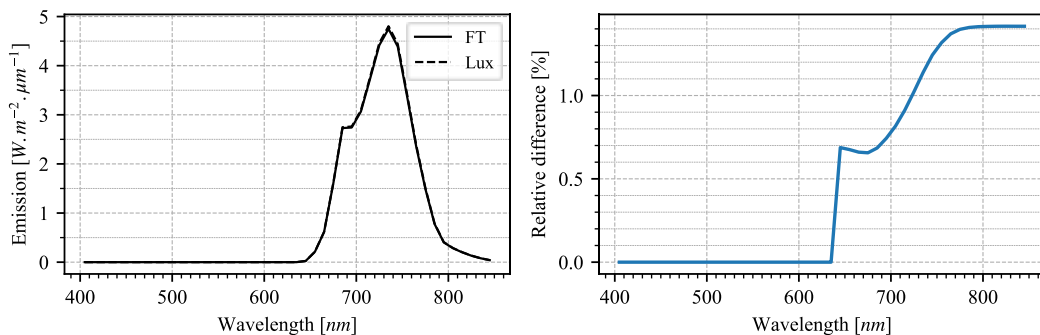


Figure 5-15: Emitted SIF of a turbid plot computed by DART-Lux compared to DART-FT (LAI = 0.5)

### 5.2.4 Discussion

The developed method takes advantage of the efficiency of DART-Lux for computing radiance images to compute the radiative budget products. It allows DART-Lux to compute most of the radiative budget components already available in DART-FT. The only case where it cannot provide results is for volumes and for spectral bands with a high single scattering albedo. However, this method is not optimal for computing the radiative budget. Indeed, the local incident radiation at each point is computed independently from the others, leading to many repetitive computations. To reduce these repetitive computations, the same light sub-paths are stored and used for all the points. This slightly improves the performance, but it is still less efficient than the forward model DART-FT.

However, it offers some advantages: 1) it is highly flexible: the user can choose to compute the radiative budget only for regions or scene elements of interest, with consideration of all the other scene elements. Therefore, in the case where the elements of interest are much smaller than the total scene, it can be more efficient than DART-FT. For instance, if one is interested



in having the SIF emission of one of the six maize plants shown in Figure 5-12, it is possible to compute it independently of the other plants (Figure 5-16) and the computation time in this case become 16 s compared to 1 min 39 s for the total scene and 54 s for DART-FT. 2) it highly parallelizable: radiative budget of different elements of the same scene can be computed independently and parallelly on several machines. 3) It can benefit from a future use of Graphics Processing Units (GPUs) for accelerating the ray tracing.

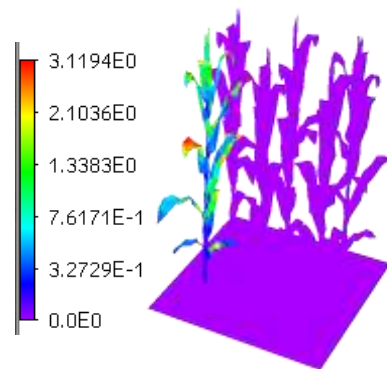


Figure 5-16: SIF emission ( $\text{W}\cdot\text{m}^{-2}\cdot\mu\text{m}^{-2}$ ) of one of the six maize plants

### 5.3 Conclusion

In this chapter, we introduced the thermal emission and radiative budget modeling in DART-Lux due to their importance in the energy balance modeling. The thermal emission modeling was introduced for scene elements simulated as facets or volumes, and allowed to simulate efficiently large-scale thermal infrared images. The radiative budget modeling is usually less efficient than DART-FT. However, it is flexible and can be efficient if the radiative budget of only a limited part of the scene is needed. It can probably be improved in the future, notably through the use of GPUs.

## Appendix 5-1: Expected value of $\hat{E}_{P,diff,1}$

$$\begin{aligned}
 \mathbb{E}[\hat{E}_{P,diff,1}] &= \frac{\pi}{N} \cdot \sum_{i=1}^N \mathbb{E}[L_{P,1}(\Omega_i)] \\
 &= \frac{\pi}{N} \cdot \sum_{i=1}^N \int_{2\pi} L_{P,1}(\Omega_i) \cdot \frac{|\Omega \cdot \vec{n}|}{\pi} \cdot d\Omega \\
 &= \int_{2\pi} L_{P,1}(\Omega_i) \cdot \frac{|\Omega \cdot \vec{n}|}{\pi} \cdot d\Omega \\
 &= E_{P,diff,1}
 \end{aligned}$$

## Appendix 5-2:

We have  $p(l) = c \cdot e^{-G(\Omega) \cdot u_l \cdot l}$  and  $\int_0^H p(l) \cdot dl = 1$ .

$$\text{Then, } c = \frac{1}{\int_0^H e^{-G(\Omega) \cdot u_l \cdot l} \cdot dl} = \frac{G(\Omega) \cdot u_l}{1 - e^{-G(\Omega) \cdot u_l \cdot H}}$$

$$\text{Therefore, } p(l) = \frac{G(\Omega) \cdot u_l \cdot e^{-G(\Omega) \cdot u_l \cdot l}}{1 - e^{-G(\Omega) \cdot u_l \cdot H}}$$

$$\text{The CDF of } p(l) \text{ is: } P(l) = \int_0^l \frac{G(\Omega) \cdot u_l \cdot e^{-G(\Omega) \cdot u_l \cdot x}}{1 - e^{-G(\Omega) \cdot u_l \cdot H}} \cdot dx = \frac{1 - e^{-G(\Omega) \cdot u_l \cdot l}}{1 - e^{-G(\Omega) \cdot u_l \cdot H}}$$

To sample a distance  $l$  from  $p(l)$  using a random number  $\xi$ :  $P(l) = \frac{1 - e^{-G(\Omega) \cdot u_l \cdot l}}{1 - e^{-G(\Omega) \cdot u_l \cdot H}} = \xi$

$$\text{Then, } l = \frac{-\ln(1 - \xi(1 - e^{-G(\Omega) \cdot u_l \cdot H}))}{G(\Omega) \cdot u_l}$$

The order 1 radiance observed by the sensor in this configuration is:

$$L_{order1}(T_1, T_2) = \int_0^H G(\Omega) \cdot u_l \cdot L_{\lambda, \Delta\lambda}(T(z)) \cdot e^{-G(\Omega) \cdot u_l \cdot z} \cdot dz$$

$$\begin{aligned}
&= \int_0^h G(\Omega) \cdot u_l \cdot L_{\lambda,\Delta\lambda}(T(z)) \cdot e^{-G(\Omega) \cdot u_l \cdot z} \cdot dz \\
&\quad + \int_h^H G(\Omega) \cdot u_l \cdot L_{\lambda,\Delta\lambda}(T(z)) \cdot e^{-G(\Omega) \cdot u_l \cdot z} \cdot dz \\
&= L_{\lambda,\Delta\lambda}(T_1)(1 - e^{-G(\Omega) \cdot u_l \cdot h}) + L_{\lambda,\Delta\lambda}(T_1)(e^{-G(\Omega) \cdot u_l \cdot H} - e^{-G(\Omega) \cdot u_l \cdot h})
\end{aligned}$$

The expected order 1 radiance computed using the sampling technique:

$$\begin{aligned}
E[\hat{L}] &= \int_0^H L_{order1}(T(z)) \cdot p(z) \cdot dz \\
&= \int_0^H L_{\lambda,\Delta\lambda}(T(z)) \cdot [1 - e^{-G(\Omega) \cdot u_l \cdot H}] \cdot \frac{G(\Omega) \cdot u_l \cdot e^{-G(\Omega) \cdot u_l \cdot z}}{1 - e^{-G(\Omega) \cdot u_l \cdot H}} \cdot dz \\
&= L_{\lambda,\Delta\lambda}(T_1) \cdot \int_0^h G(\Omega) \cdot u_l \cdot e^{-G(\Omega) \cdot u_l \cdot z} \cdot dz + L_{\lambda,\Delta\lambda}(T_2) \cdot \int_h^H G(\Omega) \cdot u_l \cdot e^{-G(\Omega) \cdot u_l \cdot z} \cdot dz \\
&= L_{\lambda,\Delta\lambda}(T_1)(1 - e^{-G(\Omega) \cdot u_l \cdot h}) + L_{\lambda,\Delta\lambda}(T_1)(e^{-G(\Omega) \cdot u_l \cdot H} - e^{-G(\Omega) \cdot u_l \cdot h}) \\
&= L_{order1}(T_1, T_2)
\end{aligned}$$

### Appendix 5-3: Variance of volume radiative budget components

Variance of  $\hat{E}_{abs}$ :

$$\begin{aligned}
var(\hat{E}_{\lambda_i,V,abs}) &= var(\hat{E}_{\lambda_i,V,in} - \hat{E}_{\lambda_i,V,out} + E_{\lambda_i,V,emis}) \\
&= var(\hat{E}_{\lambda_i,V,in}) + var(-\hat{E}_{\lambda_i,V,out}) + var(E_{\lambda_i,V,emis}) \\
&= var(\hat{E}_{\lambda_i,V,in}) + var(\hat{E}_{\lambda_i,V,out})
\end{aligned}$$

Therefore, if  $E_{\lambda_i,V,abs} \ll E_{\lambda_i,V,in}$  and  $E_{\lambda_i,V,abs} \ll E_{\lambda_i,V,out}$ ,  $var(\hat{E}_{\lambda_i,V,abs})$  becomes very high compared to the real value  $E_{\lambda_i,V,abs}$ .

Variance of  $\hat{E}_{\lambda_i,V,int}$ :

$$\begin{aligned} \text{var}(\hat{E}_{\lambda_i,V,int}) &= \text{var}\left(\frac{\hat{E}_{\lambda_i,V,abs}}{1 - \omega_{\lambda_i}}\right) \\ &= \frac{1}{(1 - \omega_{\lambda_i})^2} \left( \text{var}(\hat{E}_{\lambda_i,V,in}) + \text{var}(\hat{E}_{\lambda_i,V,out}) \right) \end{aligned}$$

Therefore,  $\text{var}(\hat{E}_{\lambda_i,V,int}) \rightarrow +\infty$  if  $\omega \rightarrow 1$

Variance of  $\hat{E}_{\lambda_i,V,scat}$ :

$$\begin{aligned} \text{var}(\hat{E}_{\lambda_i,V,scat}) &= \text{var}(\omega_{\lambda_i} \cdot \hat{E}_{\lambda_i,V,int}) \\ &= \left(\frac{\omega_{\lambda_i}}{1 - \omega_{\lambda_i}}\right)^2 \cdot \left( \text{var}(\hat{E}_{\lambda_i,V,in}) + \text{var}(\hat{E}_{\lambda_i,V,out}) \right) \end{aligned}$$

Therefore,  $\text{var}(\hat{E}_{\lambda_i,V,scat}) \rightarrow +\infty$  if  $\omega_{\lambda_i} \rightarrow 1$

## Appendix 5-4: Nomenclature

Symbol	Description	Unit
$\hat{E}_{\lambda,P,abs}$	Estimator of absorbed radiation at point $P$	$W \cdot m^{-2} \cdot \mu m^{-1}$
$\hat{E}_{\lambda,P,n}$	Estimator of incident radiation at point $P$ (order $n$ )	$W \cdot m^{-2} \cdot \mu m^{-1}$
$\hat{E}_{\lambda,P,scat}$	Estimator of scattered radiation at point $P$	$W \cdot m^{-2} \cdot \mu m^{-1}$
$\hat{E}_{\lambda,P,SIF}$	Estimator of SIF emission at point $P$	$W \cdot m^{-2} \cdot \mu m^{-1}$
$\hat{E}_{\lambda,V,abs}$	Estimator of scattered radiation at point $P$	$W \cdot m^{-2} \cdot \mu m^{-1}$
$\hat{E}_{\lambda,V,emis}$	Estimator of emitted radiation in a volume $V$	$W \cdot m^{-2} \cdot \mu m^{-1}$
$\hat{E}_{\lambda,V,int}$	Estimator of intercepted radiation in a volume $V$	$W \cdot m^{-2} \cdot \mu m^{-1}$
$\hat{E}_{\lambda,V,scat}$	Estimator of scattered radiation in a volume $V$	$W \cdot m^{-2} \cdot \mu m^{-1}$
$E_{BOA}$	Bottom of atmosphere irradiance	$W \cdot m^{-2} \cdot \mu m^{-1}$
$E_{P,1}$	First order irradiance at point $P$	$W \cdot m^{-2} \cdot \mu m^{-1}$
$E_{P,diff,1}$	First order diffuse irradiance at point $P$	$W \cdot m^{-2} \cdot \mu m^{-1}$

$E_{P,dir,1}$	First order direct irradiance at point $P$	$W.m^{-2}.\mu m^{-1}$
$E_{V,in}$	Ingoing radiation to volume $V$	$W.m^{-2}.\mu m^{-1}$
$E_{V,out}$	Outgoing radiation from volume $V$	$W.m^{-2}.\mu m^{-1}$
$E_{\lambda,P,emis}$	Emitted radiation at point $P$	$W.m^{-2}.\mu m^{-1}$
$E_{\lambda,V,emis}$	Emitted radiation at volume $V$	$W.m^{-2}.\mu m^{-1}$
$f_{sunlit}$	Fraction of sunlit leaves	-
$L_B(\lambda, T)$	Black body of temperature $T$ emitted radiance at wavelength $\lambda$	$W.m^{-2}.\mu m^{-1}.sr^{-1}$
$L_{order1}$	Order 1 emitted radiance of a volume	$W.m^{-2}.\mu m^{-1}.sr^{-1}$
$L_{\lambda,\Delta\lambda}(T)$	Emitted radiance of an object of temperature $T$ at the spectral band $(\lambda, \Delta\lambda)$	$W.m^{-2}.\mu m^{-1}.sr^{-1}$
$L_{\lambda}(T)$	Emitted radiance of an object of temperature $T$ at wavelength $\lambda$	$W.m^{-2}.\mu m^{-1}.sr^{-1}$
$M_B(T)$	Black body object of temperature $T$ thermal emission exitance	$W.m^{-2}$
$T$	Thermodynamic temperature	$K$
$T_B$	Brightness temperature	$K$
$T_P$	Thermodynamic temperature at point $P$	$K$
$\lambda_{eq}$	Equivalent wavelength	$\mu m$

# Conclusions and perspectives

This thesis was driven by the need for a comprehensive SIF model in order to link the SIF observations to the photosystem level instantaneous photosynthetic activity and to enable a better understanding and interpretation of these observations with the purpose of monitoring the photosynthesis process at different spatial and temporal scales. This is crucial for addressing some of the most imperious challenges such as climate change and the need to provide food for the increasing world population under the constraints of water scarcity and the increasing frequency of extreme weather conditions.

DART is one of the most comprehensive radiative transfer models for RS applications. Since 2017, its initial flux tracking mode (DART-FT) simulates SIF by upscaling leaf-level SIF simulated by Fluspect for canopies simulated as facets, and can provide SIF radiation budget and TOA and BOA RS observations of these canopies. Faced with the difficulty of having a complete SIF measurements dataset for a relevant comparison with a SIF radiative transfer model, we went through model-to-model comparison to assess the accuracy of the DART-FT SIF modeling. DART-FT gave results in agreement with the “reference” SIF model SCOPE/mSCOPE (1D) for horizontally homogeneous scenes and for different configurations, by approximating the turbid medium used in SCOPE with a quasi-turbid medium (*i.e.*, a cloud of facets randomly distributed). Then, DART-FT was extended to simulate SIF for vegetation represented as 3D turbid medium. This statistical representation of vegetation is widely used in RS radiative transfer models, especially for simulating large landscapes. For example, it can be useful for reducing the computational requirements for scenes simulated with a very large number of facets, or if the explicit 3D representation with facets of the simulated scene is not available (*e.g.*, only a 3D array of LAI is available). DART-FT SIF modelling for quasi-turbid medium and for turbid medium appeared to closely match. This is a kind of validation for DART-FT SIF modelling for turbid medium because DART-FT SIF modelling for quasi turbid medium has already been validated with SCOPE model.

However, the need for simulating SIF large for landscapes (e.g., a few square kilometers) driven by the advancements in the reconstruction methods of large 3D mock-ups and also the upcoming SIF satellite mission FLEX which will have a spatial resolution of 300 m, cannot be satisfied with DART-FT. Indeed, DART-FT cannot simulate large landscapes with reasonable computational resources because it tracks all radiation all over the scene which is convenient if the radiative budget of the whole scene is required, but it is not optimal for simulating images. For this reason, a more efficient mode called DART-Lux is developed. It uses a Monte Carlo bi-directional path tracing algorithm implementation from the open-source rendering engine LuxCoreRender adapted for RS applications and included in the DART framework. It can greatly decrease computation time and memory usage especially for large and complex scenes. Therefore, DART-Lux is well adapted to the simulation of large scenes. This highlights the interest to introduce the modeling of SIF and thermal emission in DART-Lux. The simulation of images in DART-Lux was extended to SIF images simulation by adapting the SIF emission equation to the bi-directional path tracing algorithm. The 3D turbid medium modeling of vegetation was also introduced, including the SIF. DART-Lux SIF modeling was assessed by comparison to DART-FT: the two modes provided results in close agreement. Computational requirements are usually much less important for DART-Lux, especially for large and complex scenes. The gain in computation time decreases if the number of spectral bands increases.

The introduction of SIF in DART-Lux allowed one to simulate SIF observations for large and complex scenes that were not possible to simulate using DART-FT. It was applied to eight realistic forest plots to evaluate the impact of the 3D structure on SIF observation by comparing 3D SIF simulations to their equivalent 1D simulations. For nadir radiance, we had large relative difference that could reach 50% especially for oblique sun directions. DART-FT radiative budget products obtained with low spectral resolution allowed one to analyze these differences. They are explained by two major reasons: 1) the canopy represented in 3D absorbs less PAR and therefore emits less SIF than 1D canopies due to clumping and shadowing effects. 2) the emitted SIF within the canopy escapes more easily from 1D canopies than from 3D canopies. Similarly, the neglect of woody elements in 3D canopies leads to an overestimation of SIF: the presence of wood elements reduces the PAR absorption by the leaves (shadowing effect) and prevents a fraction of the emitted SIF from escaping the canopy (blocking effect).

An accurate simulation of SIF requires the consideration of local meteorological parameters that influence the fluorescence quantum efficiency and therefore SIF emission. Therefore, a

simulation of the full energy budget is required including all the energy exchanges of the vegetation with its environment whether they are made via radiative or non-radiative processes. From the radiation point of view, it is essential to evaluate the energy gain of the vegetation by the incident solar radiation, and the energy loss by thermal emission. Therefore, we have introduced the modeling of the radiative budget and thermal emission in DART-Lux. Thermal emission modeling proved to be very efficient and accurate by comparison with DART-FT. Although the radiative budget modeling using the bi-directional path tracing method is less efficient than the discrete ordinates method (*i.e.*, DART-FT) for most scenes, its flexibility offers advantages. Indeed, it allows one to get the radiative budget for a set of sub-zones in the simulated scene, and this radiative budget can be calculated per type of scene element. Future improvements, notably the use of GPU acceleration, can make the implemented method more and more useful.

The remaining step towards the development of a comprehensive SIF model is the consideration of non-radiative energy exchange processes. These processes include photosynthesis, heat conduction, turbulence, etc. A 1D/ 3D energy model, called DART-EB (Energy Budget), is being developed by the DART team. In addition to the radiative energy exchanges (thermal emission, radiation budget) computed by DART, DART-EB simulates non-radiative processes. Starting from an initial guess of local temperature, the energy exchanges are computed. Obviously, the energy balance condition (*i.e.*, energy gains equal to energy loss) is not verified. Then, an iterative approach starts and local temperatures are adjusted at each iteration until convergence. (*i.e.*, reaching the energy balance). DART-EB will allow to assess the 3D temperature distribution and the multiplicative factors  $\eta$  that scale the dark-adapted leaf-level SIF emission to give steady state SIF as function of the leaf photosynthetic rate. In addition to SIF observations, thermal images will also be more accurately simulated using this physically-based approach. This is important in the frame of the preparation of the upcoming satellite missions with high spatial resolution thermal infrared sensors on-board (*i.e.*, TRISHNA mission of CNES / ISRO and LSTM mission of ESA).



## *CONCLUSIONS AND PERSPECTIVES*

## Conclusions et perspectives

Cette thèse a été motivée par le besoin d'un modèle SIF complet afin de relier les observations SIF à l'activité photosynthétique instantanée au niveau du photosystème et de permettre une meilleure compréhension et interprétation de ces observations dans le but de suivre le processus de photosynthèse à différentes échelles spatiales et temporelles. Ceci est crucial pour répondre à certains des défis les plus impérieux tels que le changement climatique et la nécessité de fournir de la nourriture à une population mondiale croissante sous les contraintes de la rareté de l'eau et de la fréquence croissante des conditions météorologiques extrêmes.

DART est l'un des modèles de transfert radiatif les plus complets pour les applications de télédétection. Depuis 2017, son mode de suivi de flux initial (DART-FT) simule la SIF en mettant à l'échelle la SIF au niveau des feuilles simulé par Fluspect pour les canopées simulées sous forme de facettes, et peut fournir un bilan radiatif de SIF et des observations de télédétections en TOA et en BOA de ces couverts. Face à la difficulté d'avoir un jeu de données complet de mesures SIF pour une comparaison pertinente avec un modèle de transfert radiatif SIF, nous sommes passés par une comparaison modèle à modèle pour évaluer la précision de la modélisation DART-FT SIF. DART-FT a donné des résultats en accord avec le modèle SIF "de référence" SCOPE/mSCOPE (1D) pour des scènes homogènes horizontalement et pour différentes configurations, en rapprochant le milieu turbide utilisé dans SCOPE avec un milieu quasi turbide (*i.e.*, un nuage de facettes réparties aléatoirement). Ensuite, DART-FT a été étendu pour simuler la SIF pour la végétation représentée sous forme de milieu turbide 3D. Cette représentation statistique de la végétation est largement utilisée dans les modèles de transfert radiatif pour la télédétection, surtout pour simuler des paysages larges. Par exemple, elle peut être utile pour réduire les besoins en ressources de calcul pour des scènes simulées avec un très grand nombre de facettes, ou si la représentation 3D explicite avec des facettes de la scène simulée n'est pas disponible (*e.g.*, seule une distribution 3D de LAI est disponible). La

modélisation de SIF de DART-FT pour le milieu quasi-turbide et pour le milieu turbide montrent une correspondance étroite. Il s'agit d'une sorte de validation pour la modélisation DART-FT SIF pour milieu turbide car la modélisation DART-FT SIF pour milieu quasi turbide a déjà été validée avec le modèle SCOPE

Cependant, le besoin de simuler la SIF pour des grands paysages (*e.g.*, quelques kilomètres carrés) porté par les progrès des méthodes de reconstruction de grandes maquettes 3D et également la prochaine mission satellite SIF FLEX qui aura une résolution spatiale de 300 m, ne peut pas être satisfait par DART-FT. En effet, DART-FT ne peut pas simuler de grands paysages avec des ressources de calcul raisonnables parce qu'il suit tous les rayons sur toute la scène, ce qui est pratique si le bilan radiatif de toute la scène est requis, mais ce n'est pas optimal pour la simulation d'images. Pour cette raison, un mode plus efficace appelé DART-Lux est développé. Il utilise une implémentation d'algorithme de traçage de chemin bidirectionnel Monte Carlo à partir du moteur de rendu open source LuxCoreRender adaptée aux applications RS et incluse dans le framework de DART. Il peut généralement réduire le temps de calcul et le besoin en mémoire, en particulier pour les scènes volumineuses et complexes. Par conséquent, DART-Lux est bien adapté à la simulation de grandes scènes. Ceci met en évidence l'intérêt d'introduire la modélisation du SIF et de l'émission thermique dans DART-Lux. La simulation d'images par DART-Lux a été étendue à la simulation d'images SIF en adaptant l'équation d'émission SIF à l'algorithme de traçage de chemin bidirectionnel. La modélisation 3D du milieu turbide de la végétation a également été introduite, y compris la SIF. DART-Lux SIF a été évalué par comparaison avec DART-FT : les deux modes ont fourni des résultats en accord étroit. Les exigences de calcul sont généralement beaucoup moins importantes pour DART-Lux, en particulier pour les scènes volumineuses et complexes. Le gain en temps de calcul diminue si le nombre de bandes spectrales augmente.

L'introduction de la SIF dans DART-Lux a permis de simuler des observations SIF pour des scènes larges et complexes qu'il n'était pas possible de simuler avec DART-FT. Il a été appliqué à huit maquettes forestières réalistes pour évaluer l'impact de la structure 3D sur l'observation SIF en comparant des simulations SIF 3D à leurs simulations 1D équivalentes. Pour la luminance au nadir, nous avons eu une grande différence relative qui pouvait atteindre 50%, en particulier pour les directions solaires obliques. Les produits de bilan radiatif DART-FT obtenus avec une faible résolution spectrale ont permis d'analyser ces différences. Elles s'expliquent par deux raisons principales : 1) la canopée représentée en 3D absorbe moins de

PAR et émet donc moins de SIF que les canopées 1D en raison des effets d'agglutination et d'ombrage. 2) la SIF émise dans la canopée s'échappe plus facilement des canopées 1D que des canopées 3D. De même, la négligence des éléments ligneux dans les canopées 3D conduit à une surestimation de la SIF : la présence d'éléments ligneux réduit l'absorption du PAR par les feuilles (effet d'ombrage) et empêche une fraction de la SIF émis de s'échapper de la canopée (effet de blocage).

Une simulation précise de la SIF nécessite la prise en compte des paramètres météorologiques locaux qui influencent l'efficacité quantique de la fluorescence et donc l'émission de SIF. Il faut donc simuler le bilan énergétique complet incluant tous les échanges énergétiques de la végétation avec son environnement qu'ils se fassent par des processus radiatifs ou non radiatifs. Du point de vue du rayonnement, il est essentiel d'évaluer le gain d'énergie de la végétation par le rayonnement solaire incident, et la perte d'énergie par émission thermique. Par conséquent, nous avons introduit la modélisation du bilan radiatif et de l'émission thermique dans DART-Lux. La modélisation des émissions thermiques s'est avérée très efficace et précise par rapport à DART-FT. Bien que la modélisation du bilan radiatif utilisant la méthode de traçage de chemin bidirectionnel soit moins efficace que la méthode des ordonnées discrètes (*i.e.*, DART-FT) pour la plupart des scènes, sa flexibilité offre des avantages. En effet, elle permet d'obtenir le bilan radiatif pour un ensemble de sous-zones de la scène simulée, et ce bilan radiatif peut être calculé par type d'élément de scène. Des améliorations futures, notamment l'utilisation de l'accélération GPU, peuvent rendre la méthode implémentée de plus en plus utile.

L'étape restante vers le développement d'un modèle SIF complet est la prise en compte des processus d'échange d'énergie non radiatifs. Ces processus incluent la photosynthèse, la conduction thermique, la turbulence, etc. Un modèle énergétique 1D/3D, appelé DART-EB (Energy Budget), est en cours de développement par l'équipe DART. En plus des échanges d'énergie radiative (émission thermique, bilan radiatif) calculés par DART, DART-EB simule des processus non radiatifs. A partir d'une estimation initiale de la température locale, les échanges d'énergie sont calculés. De toute évidence, la condition de bilan énergétique (*i.e.*, des gains d'énergie égaux à la perte d'énergie) n'est pas vérifiée. Ensuite, une approche itérative démarre et les températures locales sont ajustées à chaque itération jusqu'à convergence. (*i.e.*, atteindre l'équilibre énergétique). DART-EB permettra d'évaluer la distribution de température 3D et les facteurs multiplicatifs  $\eta$  qui pondèrent l'émission de SIF au niveau des feuilles

adaptées à l'obscurité pour donner la SIF à l'état d'équilibre en fonction du taux de photosynthèse des feuilles. En plus des observations SIF, les images thermiques seront également simulées avec plus de précision à l'aide de cette approche basée sur la physique. Ceci est important dans le cadre de la préparation des prochaines missions satellites avec des capteurs infrarouges thermiques à haute résolution spatiale embarqués (*i.e.*, la mission TRISHNA du CNES / ISRO et la mission LSTM de l'ESA).

# Bibliography

- Ač, A., Malenovský, Z., Olejníčková, J., Gallé, A., Rascher, U., & Mohammed, G. (2015). Meta-analysis assessing potential of steady-state chlorophyll fluorescence for remote sensing detection of plant water, temperature and nitrogen stress. *Remote Sensing of Environment*, *168*, 420–436. <https://doi.org/10.1016/j.rse.2015.07.022>
- Antyufeev, V. S., & Marshak, A. L. (1990). Monte Carlo method and transport equation in plant canopies. *Remote Sensing of Environment*, *31*(3), 183–191. [https://doi.org/10.1016/0034-4257\(90\)90088-4](https://doi.org/10.1016/0034-4257(90)90088-4)
- Baker, N. R. (2008). Chlorophyll Fluorescence: A Probe of Photosynthesis In Vivo. *Annual Review of Plant Biology*, *59*(1), 89–113. <https://doi.org/10.1146/annurev.arplant.59.032607.092759>
- Brewster, D. (1834). XIX. On the Colours of Natural Bodies. *Earth and Environmental Science Transactions of The Royal Society of Edinburgh*, *12*(2), 538–545. <https://doi.org/10.1017/S0080456800031203>
- Campbell, P. K. E., Huemmrich, K. F., Middleton, E. M., Ward, L. A., Julitta, T., Daughtry, C. S. T., Burkart, A., Russ, A. L., & Kustas, W. P. (2019). Diurnal and Seasonal Variations in Chlorophyll Fluorescence Associated with Photosynthesis at Leaf and Canopy Scales. *Remote Sensing*, *11*(5), Article 5. <https://doi.org/10.3390/rs11050488>
- Campbell, P. K. E., Middleton, E. M., Corp, L. A., & Kim, M. S. (2008). Contribution of chlorophyll fluorescence to the apparent vegetation reflectance. *Science of The Total Environment*, *404*(2), 433–439. <https://doi.org/10.1016/j.scitotenv.2007.11.004>
- Cogato, A., Meggio, F., De Antoni Migliorati, M., & Marinello, F. (2019). Extreme Weather Events in Agriculture: A Systematic Review. *Sustainability*, *11*(9), Article 9. <https://doi.org/10.3390/su11092547>

- Cogliati, S., Rossini, M., Julitta, T., Meroni, M., Schickling, A., Burkart, A., Pinto, F., Rascher, U., & Colombo, R. (2015). Continuous and long-term measurements of reflectance and sun-induced chlorophyll fluorescence by using novel automated field spectroscopy systems. *Remote Sensing of Environment*, *164*, 270–281.  
<https://doi.org/10.1016/j.rse.2015.03.027>
- Costa, J. M., Grant, O. M., & Chaves, M. M. (2013). Thermography to explore plant–environment interactions. *Journal of Experimental Botany*, *64*(13), 3937–3949.  
<https://doi.org/10.1093/jxb/ert029>
- Dence, T. P. (2013). A Brief Look into the Lambert W Function. *Applied Mathematics*, *4*(6), Article 6. <https://doi.org/10.4236/am.2013.46122>
- Disney, M. I., Lewis, P., & North, P. R. J. (2000). Monte Carlo ray tracing in optical canopy reflectance modelling. *Remote Sensing Reviews*, *18*(2–4), 163–196.  
<https://doi.org/10.1080/02757250009532389>
- Drusch, M., Moreno, J., Bello, U. D., Franco, R., Goulas, Y., Huth, A., Kraft, S., Middleton, E. M., Miglietta, F., Mohammed, G., Nedbal, L., Rascher, U., Schüttemeyer, D., & Verhoef, W. (2017). The FLuorescence EXplorer Mission Concept—ESA’s Earth Explorer 8. *IEEE Transactions on Geoscience and Remote Sensing*, *55*(3), 1273–1284.  
<https://doi.org/10.1109/TGRS.2016.2621820>
- Fournier, A., Daumard, F., Champagne, S., Ounis, A., Goulas, Y., & Moya, I. (2012). Effect of canopy structure on sun-induced chlorophyll fluorescence. *ISPRS Journal of Photogrammetry and Remote Sensing*, *68*, 112–120.  
<https://doi.org/10.1016/j.isprsjprs.2012.01.003>
- Frankenberg, C., Butz, A., & Toon, G. C. (2011). Disentangling chlorophyll fluorescence from atmospheric scattering effects in O<sub>2</sub> A-band spectra of reflected sun-light. *Geophysical Research Letters*, *38*(3). <https://doi.org/10.1029/2010GL045896>
- Gao, S., Huete, A., Kobayashi, H., Doody, T. M., Liu, W., Wang, Y., Zhang, Y., & Lu, X. (2022). Simulation of solar-induced chlorophyll fluorescence in a heterogeneous forest using 3-D radiative transfer modelling and airborne LiDAR. *ISPRS Journal of Photogrammetry and Remote Sensing*, *191*, 1–17.  
<https://doi.org/10.1016/j.isprsjprs.2022.07.004>

- Gascon, F., Gastellu-Etchegorry, J.-P., & Lefevre, M.-J. (2001). Radiative transfer model for simulating high-resolution satellite images. *IEEE Transactions on Geoscience and Remote Sensing*, *39*(9), 1922–1926. <https://doi.org/10.1109/36.951083>
- Gastellu-Etchegorry, J.-P., Demarez, V., Pinel, V., & Zagolski, F. (1996). Modeling radiative transfer in heterogeneous 3-D vegetation canopies. *Remote Sensing of Environment*, *58*(2), 131–156. [https://doi.org/10.1016/0034-4257\(95\)00253-7](https://doi.org/10.1016/0034-4257(95)00253-7)
- Gastellu-Etchegorry, J.-P., Lauret, N., Yin, T., Landier, L., Kallel, A., Malenovský, Z., Bitar, A. A., Aval, J., Benhmida, S., Qi, J., Medjdoub, G., Guilleux, J., Chavanon, E., Cook, B., Morton, D., Chrysoulakis, N., & Mitranka, Z. (2017). DART: Recent Advances in Remote Sensing Data Modeling With Atmosphere, Polarization, and Chlorophyll Fluorescence. *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, *10*(6), 2640–2649. <https://doi.org/10.1109/JSTARS.2017.2685528>
- Gastellu-Etchegorry, J.-P., Martin, E., & Gascon, F. (2004). DART: A 3D model for simulating satellite images and studying surface radiation budget. *International Journal of Remote Sensing*, *25*(1), 73–96. <https://doi.org/10.1080/0143116031000115166>
- Gastellu-Etchegorry, J.-P., Yin, T., Lauret, N., Cajgfinger, T., Gregoire, T., Grau, E., Feret, J.-B., Lopes, M., Guilleux, J., Dedieu, G., Malenovský, Z., Cook, B. D., Morton, D., Rubio, J., Durrieu, S., Cazanave, G., Martin, E., & Ristorcelli, T. (2015). Discrete Anisotropic Radiative Transfer (DART 5) for Modeling Airborne and Satellite Spectroradiometer and LIDAR Acquisitions of Natural and Urban Landscapes. *Remote Sensing*, *7*(2), Article 2. <https://doi.org/10.3390/rs70201667>
- Gerhards, M., Schlerf, M., Mallick, K., & Udelhoven, T. (2019). Challenges and Future Perspectives of Multi-/Hyperspectral Thermal Infrared Remote Sensing for Crop Water-Stress Detection: A Review. *Remote Sensing*, *11*(10), Article 10. <https://doi.org/10.3390/rs11101240>
- Gobron, N., Pinty, B., Verstraete, M. M., & Govaerts, Y. (1997). A semidiscrete model for the scattering of light by vegetation. *Journal of Geophysical Research: Atmospheres*, *102*(D8), 9431–9446. <https://doi.org/10.1029/96JD04013>



- Guanter, L., Frankenberg, C., Dudhia, A., Lewis, P. E., Gómez-Dans, J., Kuze, A., Suto, H., & Grainger, R. G. (2012). Retrieval and global assessment of terrestrial chlorophyll fluorescence from GOSAT space measurements. *Remote Sensing of Environment*, *121*, 236–251. <https://doi.org/10.1016/j.rse.2012.02.006>
- Guanter, L., Zhang, Y., Jung, M., Joiner, J., Voigt, M., Berry, J. A., Frankenberg, C., Huete, A. R., Zarco-Tejada, P., Lee, J.-E., Moran, M. S., Ponce-Campos, G., Beer, C., Camps-Valls, G., Buchmann, N., Gianelle, D., Klumpp, K., Cescatti, A., Baker, J. M., & Griffis, T. J. (2014). Global and time-resolved monitoring of crop photosynthesis with chlorophyll fluorescence. *Proceedings of the National Academy of Sciences*, *111*(14), E1327–E1333. <https://doi.org/10.1073/pnas.1320008111>
- Guillevic, P. C., Gastellu-Etchegorry, J.-P., Demarty, J., & Prévot, L. (2003). Thermal infrared radiative transfer within three-dimensional vegetation covers. *Journal of Geophysical Research: Atmospheres*, *108*(D8). <https://doi.org/10.1029/2002JD002247>
- Hernández-Clemente, R., North, P. R. J., Hornero, A., & Zarco-Tejada, P. J. (2017). Assessing the effects of forest health on sun-induced chlorophyll fluorescence using the FluorFLIGHT 3-D radiative transfer model to account for forest structure. *Remote Sensing of Environment*, *193*, 165–179. <https://doi.org/10.1016/j.rse.2017.02.012>
- Jabłoński, A. (1935). Über den Mechanismus der Photolumineszenz von Farbstoffphosphoren. *Zeitschrift für Physik*, *94*(1), 38–46. <https://doi.org/10.1007/BF01330795>
- Jacquemoud, S., & Baret, F. (1990). PROSPECT: A model of leaf optical properties spectra. *Remote Sensing of Environment*, *34*(2), 75–91. [https://doi.org/10.1016/0034-4257\(90\)90100-Z](https://doi.org/10.1016/0034-4257(90)90100-Z)
- Kallel, A. (2020a). Two-scale Monte Carlo ray tracing for canopy-leaf vector radiative transfer coupling. *Journal of Quantitative Spectroscopy and Radiative Transfer*, *243*, 106815. <https://doi.org/10.1016/j.jqsrt.2019.106815>
- Kallel, A. (2020b). FluLCVRT: Reflectance and fluorescence of leaf and canopy modeling based on Monte Carlo vector radiative transfer simulation. *Journal of Quantitative Spectroscopy and Radiative Transfer*, *253*, 107183. <https://doi.org/10.1016/j.jqsrt.2020.107183>

- Kallel, A., & Nilson, T. (2013). Revisiting the vegetation hot spot modeling: Case of Poisson/Binomial leaf distributions. *Remote Sensing of Environment*, *130*, 188–204. <https://doi.org/10.1016/j.rse.2012.11.018>
- Kautsky, H., Appel, W., & Amann, H. (1960). Chlorophyll fluorescence and carbon assimilation. Part XIII. The fluorescence and the photochemistry of plants. *Biochemische Zeitschrift*, *332*, 277–292.
- Kautsky, H., & Hirsch, A. (1931). Neue Versuche zur Kohlensäureassimilation. *Naturwissenschaften*, *19*(48), 964–964. <https://doi.org/10.1007/BF01516164>
- Kautsky, H., & Zedlitz, W. (1941). Fluoreszenzkurven von Chloroplasten-Grana. *Naturwissenschaften*, *29*(7), 101–102. <https://doi.org/10.1007/BF01468767>
- Kobayashi, H., & Iwabuchi, H. (2008). A coupled 1-D atmosphere and 3-D canopy radiative transfer model for canopy reflectance, light environment, and photosynthesis simulation in a heterogeneous landscape. *Remote Sensing of Environment*, *112*(1), 173–185. <https://doi.org/10.1016/j.rse.2007.04.010>
- Kuusk, A. (1985). The hot-spot effect of a uniform vegetative cover. *Soviet Journal of Remote Sensing*, *3*, 645–658.
- Lichtman, J. W., & Conchello, J.-A. (2005). Fluorescence microscopy. *Nature Methods*, *2*(12), Article 12. <https://doi.org/10.1038/nmeth817>
- Liu, X., Guanter, L., Liu, L., Damm, A., Malenovský, Z., Rascher, U., Peng, D., Du, S., & Gastellu-Etchegorry, J.-P. (2019). Downscaling of solar-induced chlorophyll fluorescence from canopy level to photosystem level using a random forest model. *Remote Sensing of Environment*, *231*, 110772. <https://doi.org/10.1016/j.rse.2018.05.035>
- Liu, Y., Kochanski, A., Baker, K. R., Mell, W., Linn, R., Paugam, R., Mandel, J., Fournier, A., Jenkins, M. A., Goodrick, S., Achtemeier, G., Zhao, F., Ottmar, R., French, N. H. F., Larkin, N., Brown, T., Hudak, A., Dickinson, M., Potter, B., ... McNamara, D. (2019). Fire behaviour and smoke modelling: Model improvement and measurement needs for next-generation smoke research and forecasting systems. *International Journal of Wildland Fire*, *28*(8), 570–588. <https://doi.org/10.1071/WF18204>

- Liu, Z., Lu, X., An, S., Heskell, M., Yang, H., & Tang, J. (2019). Advantage of multi-band solar-induced chlorophyll fluorescence to derive canopy photosynthesis in a temperate forest. *Agricultural and Forest Meteorology*, 279, 107691. <https://doi.org/10.1016/j.agrformet.2019.107691>
- Malenovský, Z., Regaieg, O., Yin, T., Lauret, N., Guilleux, J., Chavanon, E., Duran, N., Janoutová, R., Delavois, A., Meynier, J., Medjdoub, G., Yang, P., van der Tol, C., Morton, D., Cook, B. D., & Gastellu-Etchegorry, J.-P. (2021). Discrete anisotropic radiative transfer modelling of solar-induced chlorophyll fluorescence: Structural impacts in geometrically explicit vegetation canopies. *Remote Sensing of Environment*, 263, 112564. <https://doi.org/10.1016/j.rse.2021.112564>
- McAlister, E. D., & Myers, J. (1940). Time Course of Photosynthesis and Fluorescence. *Science*, 92(2385), 241–243. <https://doi.org/10.1126/science.92.2385.241>
- McGrattan, K. B., McDermott, R. J., Weinschenk, C. G., & Forney, G. P. (2013). Fire Dynamics Simulator, Technical Reference Guide, Sixth Edition. *NIST*. <https://www.nist.gov/publications/fire-dynamics-simulator-technical-reference-guide-sixth-edition>
- Mell, W., Jenkins, M. A., Gould, J., Cheney, P., Mell, W., Jenkins, M. A., Gould, J., & Cheney, P. (2007). A physics-based approach to modelling grassland fires. *International Journal of Wildland Fire*, 16(1), 1–22. <https://doi.org/10.1071/WF06002>
- Moya, I., Camenen, L., Evain, S., Goulas, Y., Cerovic, Z. G., Latouche, G., Flexas, J., & Ounis, A. (2004). A new instrument for passive remote sensing: 1. Measurements of sunlight-induced chlorophyll fluorescence. *Remote Sensing of Environment*, 91(2), 186–197. <https://doi.org/10.1016/j.rse.2004.02.012>
- Müller, N. J. C. (1874). Beziehungen zwischen assimilation, absorption und fluoreszenz im chlorophyll des lebenden blattes. *Jahrb Wiss Bo*, 9, 42–49.
- North, P. R. J. (1996). Three-dimensional forest light interaction model using a Monte Carlo method. *IEEE Transactions on Geoscience and Remote Sensing*, 34(4), 946–956. <https://doi.org/10.1109/36.508411>
- Paugam, R., Wooster, M. J., & Roberts, G. (2013). Use of Handheld Thermal Imager Data for Airborne Mapping of Fire Radiative Power and Energy and Flame Front Rate of

- Spread. *IEEE Transactions on Geoscience and Remote Sensing*, 51(6), 3385–3399.  
<https://doi.org/10.1109/TGRS.2012.2220368>
- Pedros, R., Goulas, Y., Jacquemoud, S., Louis, J., & Moya, I. (2010). FluorMODleaf: A new leaf fluorescence emission model based on the PROSPECT model. *Remote Sensing of Environment*, 114(1), 155–167. <https://doi.org/10.1016/j.rse.2009.08.019>
- Porcar-Castell, A., Tyystjärvi, E., Atherton, J., van der Tol, C., Flexas, J., Pfündel, E. E., Moreno, J., Frankenberg, C., & Berry, J. A. (2014). Linking chlorophyll a fluorescence to photosynthesis for remote sensing applications: Mechanisms and challenges. *Journal of Experimental Botany*, 65(15), 4065–4095.  
<https://doi.org/10.1093/jxb/eru191>
- Regaieg, O., Yin, T., Malenovský, Z., Cook, B. D., Morton, D. C., & Gastellu-Etchegorry, J.-P. (2021). Assessing impacts of canopy 3D structure on chlorophyll fluorescence radiance and radiative budget of deciduous forest stands using DART. *Remote Sensing of Environment*, 265, 112673. <https://doi.org/10.1016/j.rse.2021.112673>
- Rossini, M., Nedbal, L., Guanter, L., Ač, A., Alonso, L., Burkart, A., Cogliati, S., Colombo, R., Damm, A., Drusch, M., Hanus, J., Janoutova, R., Julitta, T., Kokkalis, P., Moreno, J., Novotny, J., Panigada, C., Pinto, F., Schickling, A., ... Rascher, U. (2015). Red and far red Sun-induced chlorophyll fluorescence as a measure of plant photosynthesis. *Geophysical Research Letters*, 42(6), 1632–1639.  
<https://doi.org/10.1002/2014GL062943>
- Sakai, Y., Kobayashi, H., & Kato, T. (2020). FLiES-SIF version 1.0: Three-dimensional radiative transfer model for estimating solar induced fluorescence. *Geoscientific Model Development*, 13(9), 4041–4066. <https://doi.org/10.5194/gmd-13-4041-2020>
- Stokes, G. G. (1852). XXX. On the change of refrangibility of light. *Philosophical Transactions of the Royal Society of London*, 142, 463–562.  
<https://doi.org/10.1098/rstl.1852.0022>
- Suárez, L., Zarco-Tejada, P. J., Berni, J. A. J., González-Dugo, V., & Fereres, E. (2009). Modelling PRI for water stress detection using radiative transfer models. *Remote Sensing of Environment*, 113(4), 730–744. <https://doi.org/10.1016/j.rse.2008.12.001>

- Sušila, P., & Nauš, J. (2007). A Monte Carlo study of the chlorophyll fluorescence emission and its effect on the leaf spectral reflectance and transmittance under various conditions. *Photochemical & Photobiological Sciences*, 6(8), 894–902. <https://doi.org/10.1039/B618315H>
- Valeur, B. (2012a). Characteristics of Fluorescence Emission. In *Molecular Fluorescence* (pp. 53–74). John Wiley & Sons, Ltd. <https://doi.org/10.1002/9783527650002.ch3>
- Valeur, B. (2012b). Introduction. In *Molecular Fluorescence* (pp. 1–30). John Wiley & Sons, Ltd. <https://doi.org/10.1002/9783527650002.ch1>
- van der Tol, C., Verhoef, W., Timmermans, J., Verhoef, A., & Su, Z. (2009). An integrated model of soil-canopy spectral radiances, photosynthesis, fluorescence, temperature and energy balance. *Biogeosciences*, 6(12), 3109–3129. <https://doi.org/10.5194/bg-6-3109-2009>
- Vilfan, N., van der Tol, C., Muller, O., Rascher, U., & Verhoef, W. (2016). Fluspect-B: A model for leaf fluorescence, reflectance and transmittance spectra. *Remote Sensing of Environment*, 186, 596–615. <https://doi.org/10.1016/j.rse.2016.09.017>
- Vilfan, N., Van der Tol, C., Yang, P., Wyber, R., Malenovský, Z., Robinson, S. A., & Verhoef, W. (2018). Extending Fluspect to simulate xanthophyll driven leaf reflectance dynamics. *Remote Sensing of Environment*, 211, 345–356. <https://doi.org/10.1016/j.rse.2018.04.012>
- Wang, Y., & Gastellu-Etchegorry, J.-P. (2021). Accurate and fast simulation of remote sensing images at top of atmosphere with DART-Lux. *Remote Sensing of Environment*, 256, 112311. <https://doi.org/10.1016/j.rse.2021.112311>
- Wang, Y., Kallel, A., Yang, X., Regaieg, O., Lauret, N., Guilleux, J., Chavanon, E., & Gastellu-Etchegorry, J.-P. (2022). DART-Lux: An unbiased and rapid Monte Carlo radiative transfer method for simulating remote sensing images. *Remote Sensing of Environment*, 274, 112973. <https://doi.org/10.1016/j.rse.2022.112973>
- Yang, P., van der Tol, C., Campbell, P. K. E., & Middleton, E. M. (2021). Unraveling the physical and physiological basis for the solar- induced chlorophyll fluorescence and photosynthesis relationship using continuous leaf and canopy measurements of a corn crop. *Biogeosciences*, 18(2), 441–465. <https://doi.org/10.5194/bg-18-441-2021>

- Yang, P., Verhoef, W., & van der Tol, C. (2017). The mSCOPE model: A simple adaptation to the SCOPE model to describe reflectance, fluorescence and photosynthesis of vertically heterogeneous canopies. *Remote Sensing of Environment*, *201*, 1–11. <https://doi.org/10.1016/j.rse.2017.08.029>
- Yang, X., Wang, Y., Yin, T., Wang, C., Lauret, N., Regaieg, O., Xi, X., & Gastellu-Etchegorry, J. P. (2022). Comprehensive LiDAR simulation with efficient physically-based DART-Lux model (I): Theory, novelty, and consistency validation. *Remote Sensing of Environment*, *272*, 112952. <https://doi.org/10.1016/j.rse.2022.112952>
- Yin, T., Cook, B. D., & Morton, D. C. (2022). Three-dimensional estimation of deciduous forest canopy structure and leaf area using multi-directional, leaf-on and leaf-off airborne lidar data. *Agricultural and Forest Meteorology*, *314*, 108781. <https://doi.org/10.1016/j.agrformet.2021.108781>
- Yin, T., Gastellu-Etchegorry, J.-P., Lauret, N., Grau, E., & Rubio, J. (2013). A new approach of direction discretization and oversampling for 3D anisotropic radiative transfer modeling. *Remote Sensing of Environment*, *135*, 213–223. <https://doi.org/10.1016/j.rse.2013.03.030>
- Zhao, F., Dai, X., Verhoef, W., Guo, Y., van der Tol, C., Li, Y., & Huang, Y. (2016). FluorWPS: A Monte Carlo ray-tracing model to compute sun-induced chlorophyll fluorescence of three-dimensional canopy. *Remote Sensing of Environment*, *187*, 385–399. <https://doi.org/10.1016/j.rse.2016.10.036>
- Zhao, F., Li, Y., Dai, X., Verhoef, W., Guo, Y., Shang, H., Gu, X., Huang, Y., Yu, T., & Huang, J. (2015). Simulated impact of sensor field of view and distance on field measurements of bidirectional reflectance factors for row crops. *Remote Sensing of Environment*, *156*, 129–142. <https://doi.org/10.1016/j.rse.2014.09.011>