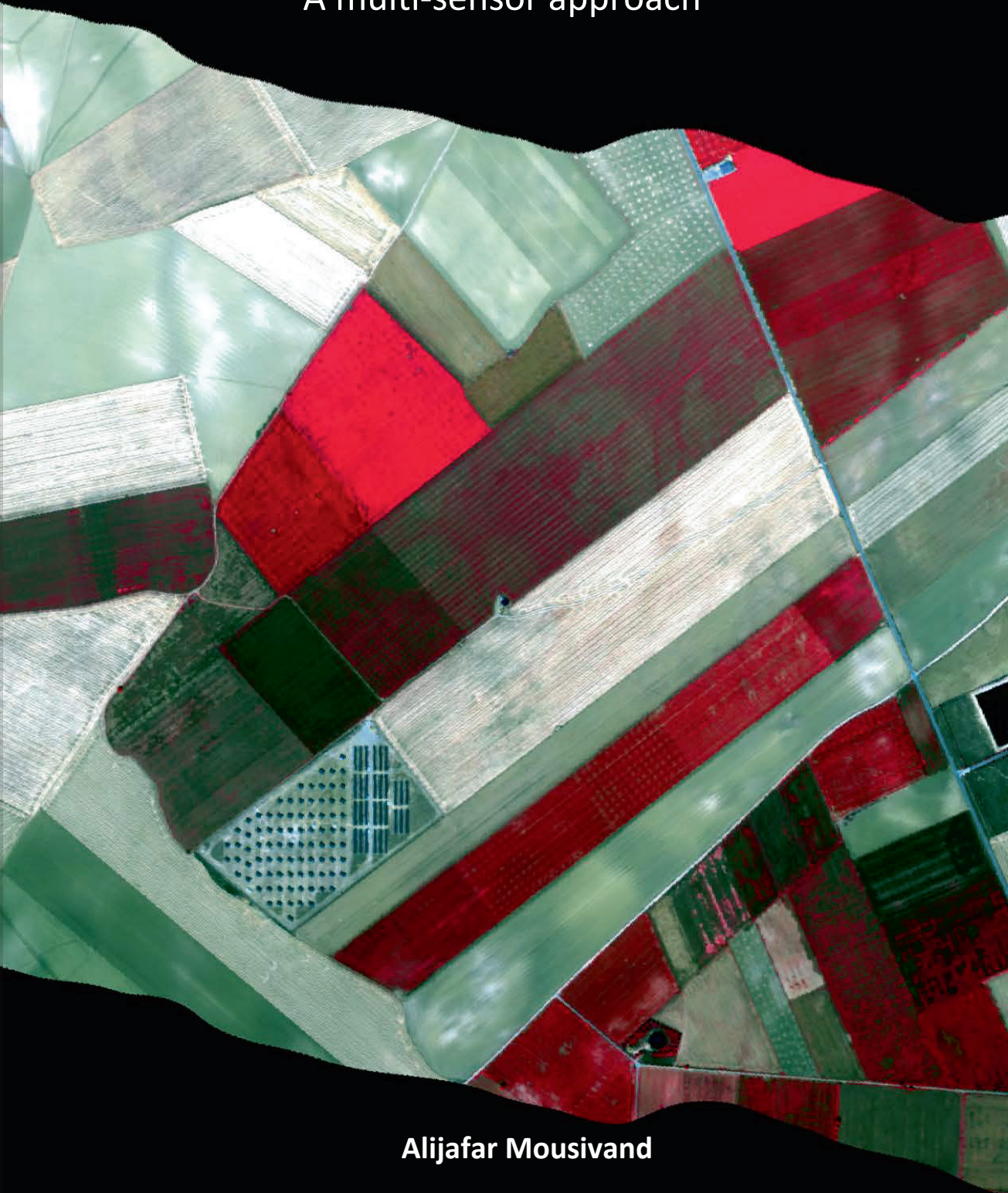


Retrieval of vegetation properties using Top of Atmosphere radiometric data

A multi-sensor approach



Alijafar Mousivand

Retrieval of vegetation properties using Top of Atmosphere radiometric data: A multi-sensor approach

Retrieval of vegetation properties using Top of Atmosphere radiometric data: A multi-sensor approach

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Front & Back: Airborne imagery from the Compact Airborne Spectrographic Imager (CASI) over the Barrax, Spain (20-06-2009) with 1.5 meter spatial resolution. Band combination: R(750 nm), G(649 nm) and B(549 nm).

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Summary

Vegetation is the main source of primary production and plays an important role in modeling the exchanges of energy and mass of carbon, oxygen and water between the earth and the atmosphere. Mapping and monitoring of vegetation canopies are crucial for various applications including agro-ecosystem models, climatology modeling, crop growth modeling and vegetation productivity modeling. The reflected radiance from vegetation carries information about chemical and bio-geophysical vegetation characteristics. Leaf area index (LAI), chlorophyll content and fraction of vegetation cover (fCover) are among the most important vegetation properties that can be retrieved from satellite observations. Over the past decades, considerable effort has been given toward improving vegetation properties retrieval from remotely sensed data. A number of satellite observations are currently being utilized to retrieve vegetation characteristics in a diverse range of spatial and temporal resolutions and new ones will become available soon with an unprecedented capacity to quantify vegetation properties. The accurate vegetation variable retrieval depends on three issues: radiometric data quality, forward radiance modeling and parametrization and regularization. The major goal of this contribution is to improve vegetation properties retrieval from top of atmosphere optical satellite observations, given the richness of current and near-future sources of optical remote sensing data. The first part of this contribution deals with model parameterization for variable retrieval and determining retrievable variables through sensitivity analysis. The sensitivity of top of atmosphere radiance and surface reflectance of a soil-vegetation system to input biophysical and biochemical variables is estimated using the coupled Soil-Leaf-Canopy radiative transfer model SLC and MODTRAN. This study also proposes an improvement to the design and sampling of screening methods for efficient sensitivity analysis of computationally expensive models. The results demonstrated high correlation between the proposed improvement (with only modest computational demands) against variance-based global sensitivity analysis in determining the most influential and non-influential variables.

The second part of this contribution provides a proof of concept for a multi-temporal, multi-sensor approach to retrieve biophysical and biochemical vegetation variables using spectral-directional radiometric data. The approach is designed for the exploitation of a temporal sequence constructed by combining data acquired by different sensors over time. Focus is given to the retrieval of three important vegetation variables; LAI, fCover and chlorophyll content over the agricultural test site in Barrax, Spain. A variety of different satellite observations including, CHRIS-Proba, Landsat TM and ASTER are used to invert the coupled surface-atmosphere SLC-MODTRAN radiative transfer model. This thesis presents an overview of the results and challenges in utilizing the multi-temporal, multi-sensor approach and the Bayesian inversion technique in the retrieval of terrestrial vegetation properties. It was shown that the approach is capable of dealing with a diversity of optical sensors by exploiting heterogeneous radiometric data

and allows for having frequent updates of vegetation biophysical and biochemical products over time. Moreover, the results showed that integrating information from different sensors improves the retrieval of vegetation variables compared to the case of single sensor retrievals.

The last part of this contribution is devoted to the investigation of the topographic effects on top of atmosphere radiance modeling and variable retrieval. To account for such effects, this study presents an extension of “*the four-stream radiative transfer theory*” previously proposed by Verhoef and Bach (2003b, 2007, 2012). The extension is mainly focused on two aspects in top of atmosphere radiance modeling. First, the study gives a detailed account of the main topography-induced effects on top of atmosphere radiance modeling and the relevant equations are given. Second, a new formulation is proposed for the derivation of the six atmospheric coefficients using MODTRAN in order to make it more computationally efficient, as well as to avoid using zero surface albedo which causes some miscalculations in the results. It was demonstrated that the topographic effect has to be taken into account in variable retrieval and the approach presented in this thesis can be used to model such effects on top of atmosphere radiance over rugged terrain.

Samenvatting

Vegetatie is de voornaamste bron van primaire productie en speelt een belangrijke rol in het modelleren van wisselingen van energie en massa van koolstof, zuurstof en water tussen aarde en atmosfeer. Het in kaart brengen en monitoren van het vegetatiedek is cruciaal voor verscheidene toepassingen zoals agro-ecosysteemmodellen, klimatologie-modellering, groeimodellering van gewassen en productiviteitsmodellering van vegetatie. De gereflecteerde radiatie van vegetatie bevat informatie over chemische en biochemische vegetatie-eigenschappen. Leaf area index (LAI), chlorofylgehalte en fraction of vegetation cover (fCover) zijn enkele van de meest belangrijke vegetatie-eigenschappen die kunnen worden verkregen uit waarnemingen vanuit satellieten.

Gedurende de afgelopen decennia zijn aanzienlijke inspanningen besteed aan het verbeteren van het verkrijgen van vegetatie-eigenschappen uit remote sensing. Een aantal waarnemingen vanuit satellieten wordt momenteel gebruikt voor het verkrijgen van vegetatiekarakteristieken met een diverse verscheidenheid aan ruimtelijke en temporele resoluties en nieuwe waarnemingen zullen op korte termijn beschikbaar komen resulterend in een ongekend vermogen om vegetatie-eigenschappen te kwantificeren. Het nauwkeurig verkrijgen van vegetatievariabelen hangt af van drie kwesties: radiometrische datakwaliteit, voorwaartse radiatie modellering en parametrisering en reglementering. Het voornaamste doel van deze bijdrage is het verbeteren van het verkrijgen van vegetatie-eigenschappen uit top-van-atmosfeer optische waarnemingen vanuit satellieten, rekening houdend met de weelde van huidige en binnenkort te verwachten bronnen op het gebied van optische remote sensing. Het eerste gedeelte van deze bijdrage gaat in op de modelparametrisatie voor variabelretrieval en het bepalen van verkrijgbare variabelen door middel van een gevoeligheidsanalyse. De gevoeligheid van top-van-atmosfeer radiatie en oppervlaktereflectie van een grond-vegetatie systeem op biofysische en biochemische input variabelen is vastgesteld waarbij gebruik is gemaakt van de koppeling tussen het Soil-Leaf-Canopy radiative transfer model SLC en MODTRAN. Dit onderzoek biedt ook een verbetering op het ontwerp en sampling van screening methodieken voor efficiënte gevoeligheidsanalyses van rekenkundig kostbare modellen. De resultaten tonen hoge correlatie aan tussen de voorgestelde verbetering (met bescheiden rekenkundige eisen) en de variantie-gebaseerde globale gevoeligheidsanalyse bij het bepalen van de meest invloedrijke en niet-invloedrijke variabelen.

Het tweede gedeelte van deze bijdrage biedt een “proof of concept” voor een multi-temporele, multi-sensor aanpak voor het verkrijgen van biofysische en biochemische vegetatievariabelen gebruikmakend van spectraal-directioneel radiometrische data. De aanpak is dusdanig ontworpen dat het gebruik kan maken van een tijdsreeks bestaande uit een combinatie van data afkomstig uit verschillende sensoren over tijd. Aandacht is besteed aan de retrieval van drie belangrijke vegetatievariabelen; LAI, fCover en chlorofylgehalte over het agrarische testgebied in Barrax, Spanje. Een variëteit aan verschillende waarnemingen vanuit satellieten waaronder CHRIS-Proba, Landsat TM en ASTER

zijn gebruikt om de gekoppelde oppervlakte-atmosfeer SLC-MODTRAN radiative transfer model te inverteren. Dit proefschrift geeft een overzicht weer van de resultaten en uitdagingen in het toepassen van de multi-temporele, multi-sensor aanpak en de Bayesische inversie techniek in de retrieval van aardse vegetatie-eigenschappen. Er wordt bewezen dat de aanpak in staat is om om te gaan met een diversiteit aan optische sensoren door middel van het exploiteren van heterogene radiometrische data en tevens frequente updates van vegetatie-gerelateerde biofysische en biochemische producten over tijd te verwerken. Bovendien laten de resultaten zien dat het integreren van informatie komende uit verschillende sensoren de retrieval van vegetatievariabelen verbetert in vergelijking tot het geval van retrieval uit een enkele sensor.

Het laatste gedeelte van deze bijdrage is toegewijd aan het onderzoek naar de topografische effecten op de modellering van top-van-atmosfeer radiatie en variabelretrieval. Om rekening te houden met dit soort effecten biedt dit proefschrift een uitbreiding op de “four-stream radiative transfer theory” welke eerder was voorgesteld door Verhoef and Bach (2003b, 2007, 2012). De uitbreiding is voornamelijk geconcentreerd op twee aspecten in top-van-atmosfeer radiatiemodellering. Ten eerste geeft dit onderzoek een gedetailleerd beeld van de voornaamste topografisch-geïnduceerde effecten op de top-van-atmosfeer radiatiemodellering en de bijbehorende relevante vergelijkingen. Ten tweede is een nieuwe formulering voorgesteld voor de afleiding van de zes atmosferische coëfficiënten met behulp van MODTRAN om zo het proces rekenkundig meer efficiënt te maken, tevens om te voorkomen dat een zero oppervlakte albedo wordt gebruikt welke miscalculaties in de resultaten kan veroorzaken. Het is aangetoond dat het topografische effect moet worden meegenomen in variabelretrieval en de aanpak geïntroduceerd in dit proefschrift kan worden gebruikt om zulke effecten op top-van-atmosfeer radiatie over ruig terrein te modelleren.

Preface

Looking back and reflecting on my PhD journey, I can now say that it has been a very unique experience, a journey through both difficult moments and rewarding ones and filled with valuable lessons that shaped me and my future path. Many people contributed to the successful completion of this thesis in different ways, for which I am sincerely grateful.

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1

Introduction

1.1. Background

Vegetation converts solar light into chemical energy through photosynthesis on which all animal species on the planet are ultimately directly or indirectly dependent. The photosynthesis process is not only vital for food production but also by absorbing atmospheric carbon dioxide it plays a crucial role as a terrestrial carbon sink. Even small changes in global vegetation photosynthesis may affect the carbon sequestration on Earth and hence influence the climate change (Luyssaert et al., 2007). Vegetation regulates the flow of energy and mass through the carbon, nitrogen and water cycles in local and global energy balances.

Vegetation mapping and monitoring are in high demand for a wide range of applications such as agro-ecosystem models, carbon cycle, climatology modeling, crop growth modeling and vegetation productivity modeling (Baret et al., 2007; D'Urso et al., 2009; Goel, 1988; Menenti et al., 2005; North, 2002; Sellers et al., 1997). These models require information on the vegetation biophysical and biochemical properties to represent radiation, water, heat and gas exchanges with the atmosphere and the background soil (Monteith and Unsworth, 1990). Leaf area index (LAI), chlorophyll content and fraction of vegetation cover (fCover) are among the most important vegetation properties used in these models. LAI quantifies the amount of green foliage in the canopy, chlorophyll content indicates how much photosynthesis the canopy is capable of, and fCover presents the fraction of background soil covered by vegetation. The knowledge of such variables gives insight into the vegetation health, growth stage and productivity which is, in turn, critical to determine the extent and quality of vegetation and to study the long-term dynamics of terrestrial vegetation.

Vegetation biophysical and biochemical variables can be either measured directly or estimated indirectly (remotely). Although the direct measurements are generally deemed the most accurate way of collecting such information, they are often destructive, labor demanding and time consuming and cannot be applied over large areas due to the temporal and spatial variability of vegetation (Weiss et al., 2004). Instead, indirect measurements offer a faster and simpler way to estimate vegetation properties using relevant instruments (e.g. LiCor2000 for LAI estimation). However, indirect ground-based methods are still prone partially to the problems discussed with the direct measurements for large scale data collection. Optical remote sensing, due to its synoptic view and repetitive measurements, provides a unique tool to retrieve vegetation properties as well as to monitor and map changes in the state and condition of vegetation canopies on regional to global scales (Menenti et al., 2005; Myneni et al., 2002). Optical remote sensors record the radiation from the visible through the short-wave infrared (SWIR) wavelengths (i.e. 400 to 2500 nm), which is mainly dominated by reflected solar radiance by objects. Thermal emission is small in this region so that it can be neglected. The reflected radiation carries information about the observed vegetation scenes and their physical and chemical characteristics.

Remote sensing is indeed an indirect measurement in which vegetation characteristics have to be retrieved from radiometric data. An enormous amount of work has been devoted to the retrieval of vegetation characteristics from remotely sensed data (e.g. (Baret and Buis, 2008; Liang, 2004)). The retrieval approaches range from establishing a simple relationship between the variables of interest and vegetation indices to

the inversion of sophisticated physically-based radiative transfer models (Kimes, 2000; Knyazikhin and Martonchik, 1998; Verstraete et al., 1996). The approaches based on empirical-statistical relationships (e.g. between NDVI and LAI) are simple and easy to implement. However, they are limited to the conditions for which they were trained and their transferability to other conditions is highly restricted due to their site-, time- and sensor-specific nature (Gobron and Verstraete, 1997). Contrariwise, approaches relying on physically-based models do not need training and calibration and, therefore, they are readily transferable to other areas and conditions. In such an approach, a physically-based model (e.g. radiative transfer) simulating spectral reflectance/radiance has to be inverted against satellite measurements. The ill-posed nature of physically-based model inversions is often considered as the main drawback in applying such models for retrieval.

Several satellite missions are currently being used to retrieve vegetation characteristics in a wide range of spatial and temporal resolutions. Moreover, new generations of high to moderate spatial resolution space-borne sensors collecting radiometric data in several narrow spectral bands within a short re-visit time, both hyperspectral (e.g. En-Map) and multi-spectral (e.g. Sentinel 2) are expected to become available soon with an unprecedented capacity to measure vegetation properties. Such a rich spectral and angular sampling of vegetated surfaces offers a great potential for more accurate and temporally frequent vegetation products.

1.2. Vegetation variable retrieval limitations

Over the last decades, a great deal of effort has been done to improve the quality and quantity of vegetation characteristics retrieved from remotely sensed data (Baret and Buis, 2008; Goel, 1988; Knyazikhin and Martonchik, 1998; Liang, 2004; Myneni et al., 2002; Sellers et al., 1997; Verstraete, 1994; Weiss et al., 2000). This has led to the development of a number of canopy reflectance models and algorithms to retrieve biophysical and biochemical properties of vegetation. Vegetation products are nowadays produced regularly on global and regional scales by a variety of optical satellite missions (Baret et al., 2007). For instance, terrestrial land surface properties including vegetation products such as LAI, fCover are regularly produced by available coarse spatial resolution sensors like MODIS and VEGETATION. These biophysical variables are produced globally at different temporal and spatial sampling intervals (e.g. 1-km MODIS 8-day LAI and 1-km VEGETATION 10-day LAI) (Baret et al., 2007). There also exist several optical missions at high to intermediate spatial resolutions (1-100m) designed to obtain appropriate vegetation products. Despite the considerable effort invested in the development of new retrieval methods and the improvement in the performance of such methods, they still present limitations due to a number of issues. We shall discuss these limitations below.

1.2.1. Top-Of-Canopy reflectance retrieval approach

The quality of the vegetation products retrieved through physically-based model inversion depends critically on the quality of sensor measurements and model simulations. The physically-based model has to be accurate enough to allow realistic simulation of sensor measurements. Discrepancy between the measured and simulated radiative quan-

tities due to inaccuracy of the model introduces serious difficulties and challenges into the retrieval problem. Most attention has been given to the retrieval of vegetation properties from Top-Of-Canopy (TOC) reflectance and only a few studies investigated the potential of Top-Of-Atmosphere (TOA) radiance in retrieving vegetation characteristics (e.g. (Laurent et al., 2011a)). In order to convert the raw radiance recorded by a sensor to TOC reflectance, it is necessary to apply preprocessing and corrections on the satellite radiometric data. This involves a series of corrections such as atmospheric correction, angular effects and topographic (illumination) corrections. These preprocessing and corrections are often done separately in a sequence and commonly independent of one another. For instance, atmospheric correction is often done with an average typical atmospheric profile and Lambertian surface reflection assumptions. The latter is not the case, however, where natural surfaces and even the atmosphere itself behave anisotropically (Rahman et al., 1993b). In addition to error propagation caused by these corrections, due to the inter-related effects of the atmosphere and the surface, independent processing would not reflect the physical interaction of the system (Laurent et al., 2011a).

A further drawback of the approaches based on TOC reflectance is that they only use a single reflectance factor which is mostly the bi-directional reflectance factor (BRF). The BRF simulated by radiative transfer models is inverted versus TOC reflectance obtained from satellite measurements. However, in practice, the reflectance factor that can be actually derived from satellite imageries, after applying such corrections, is the hemispherical-conical reflectance factor (HCRF). The HCRF can be considered as an approximation of the hemispherical-directional reflectance factor (HDRF) under the assumption that directional effects within the instantaneous field of view of the sensor are negligible (Schaepman-Strub et al., 2006). This inconsistency between the reflectance factors introduces some uncertainty into the retrieval procedure.

1.2.2. Top-Of-Atmosphere radiance retrieval approach

A practical alternative to avoid aforementioned problems with TOC reflectance retrieval approach is to shift from top of canopy level to top of atmosphere. This implies the integration of various corrections in the radiance simulation procedure through coupled surface-atmosphere radiative transfer model. Coupling surface and atmosphere radiative transfer models to simulate at-sensor radiance has been described by many authors (Fourty and Baret, 1997; Guanter and Kaufmann, 2009; Isaacs and Vogelmann, 1988; Laurent et al., 2011b; Rahman et al., 1993b; Schott, 2007; Verhoef and Bach, 2003b, 2007, 2012; Zhang et al., 2010). Among them, the four-stream approach proposed by Verhoef and Bach (2003b, 2007) is a good example of a trade-off between computational efficiency and accuracy. The approach has been validated against both synthetic data and satellite measurements (Verhoef and Bach, 2007; Widlowski et al., 2007). The approach was initially developed for a flat terrain and recently was extended to account for sloped terrains as well (Verhoef and Bach, 2012). However, the approach only accounts for the slope of the target pixel and the topographic effects (e.g. cast shadow) caused by the neighboring features are not taken into account. In the case of variable retrieval using TOA radiance, neglecting topographic effects is likely to lead to serious problems in particular over rugged terrain and for pixels not fully exposed to the sun and those located

partly or fully in shadow.

1.2.3. Model parameterization and retrievable variables

Canopy reflectance is a complex function of the interaction of solar radiation with different canopy components. Radiative transfer models often require a large number of input variables and parameters to simulate reflectance/radiance of vegetation canopies. Physically-based variable retrieval approach inverts such radiative transfer models against satellite observations. Because of the limited number of independent observations, it is not often practical to retrieve all the input variables concurrently (Kimes, 2000; Menenti et al., 2005). Therefore, a reliable retrieval is only possible by applying additional assumptions and constraints on the input variables. It is also known that some input variables have a limited influence on the output radiance and reflectance. A typical practice is to keep only a few free variables and fix the other inputs to a value within their plausible range of variation. Therefore, it is important to explore which variables are the most influential (i.e. likely to be retrievable) on the radiometric data at hand and which ones can be assumed fixed without affecting the retrieval performance considerably. For a variable to be retrievable, the measurements must be sensitive to that variable. To this end, following considerations have to be made prior to the inversion; (I) are the model assumptions robust enough or the model is dependent on fragile assumptions?, (II) which input parameters/variables are the most deserving of further analysis?, (III) to what extent we can safely fix model inputs or simplify them?, and (IV) what are the interesting and critical regions of the spectrum for a certain parameter or a group of parameters?

For given variables, a sensitivity study quantifies how much each variable contributes to the observed spectral radiance. This indicates wavelength dependency and identifies spectral ranges (bands) containing most information about specific variables. Identifying which target properties control spectral radiance at a given wavelength and which ones have a negligible influence on spectral radiance at the same wavelength is very useful in the retrieval problem. Most studies simply focus on the variables of interest and fix the other inputs without considering the effect of the fixed variables on the variable retrieval performance (Atzberger and Richter, 2012; Gonzalez-Sanpedro et al., 2008). There are fewer studies where a sensitivity analysis has been performed to identify which variables may be kept constant during the inversion. Moreover, the sensitivity analysis methods are limited to One (parameter) At a Time (OAT) methods (Asner et al., 2000; Bach and Verhoef, 2003; Barton and North, 2001; Bicheron and Leroy, 1999; Laurent et al., 2011a; Peres and DaCamara, 2004; Privette et al., 1994; Wang et al., 2008; Yao et al., 2008) because of simplicity and limited computational time. Although not extensive, the literature does contain a few studies that applied global sensitivity analysis methods to quantify the sensitivity of output radiance/reflectance to input variables of interest (Bacour et al., 2002; Ceccato et al., 2002; Morris et al., 2008; Pingheng and Quan, 2011). Despite the OAT methods, global sensitivity analysis methods provide accurate sensitivity measures in which simultaneous parameter variation and robust statistical measures are combined. However, they are computationally expensive and complex because of the required large number of model evaluations (Saltelli et al., 2008). This is indeed important when coupled surface-atmosphere radiative transfer models are used,

since the computational burden of such a coupled model can be considerable. Therefore, there is a need to design methods to estimate sensitivities with an accuracy comparable to sophisticated global methods but with much less computational load.

1.2.4. Sensor-specific retrieval limitations

The variety of available retrieved vegetation products from different space agencies continues to expand as more satellite missions become available and due to the increased demand for better temporal and spatial vegetation products. However, most of the available satellite vegetation products are still sensor-specific and rely on using measurements from a single sensor. Since each sensor provides its own products based upon its specifications, dedicated process chain, assumptions and simplifications, this leads to the generation of various (somewhat different) products from individual sensors (Quaife et al., 2008). The exploitation of such information from various products to determine the most appropriate product for a certain application becomes difficult and cumbersome. For instance, pre-calculated look-up-tables (LUT) of a three-dimensional radiative transfer model are used to retrieve LAI/FPAR from MODIS spectral bands. In the case of failure of the main algorithm to find a solution, the backup method based on the NDVI and LAI/FPAR relationship is utilized together with a biome classification map (Myneni et al., 2002). For SPOT-VEGETATION sensor, the retrieval algorithm is based on the training of neural networks over the SAIL+PROSPECT radiative transfer model simulations for each biophysical variable (Baret et al., 2007). There is a number of approaches, in the literature, to retrieve vegetation properties from other satellite missions as well. The given examples illustrate the diversity of radiative transfer models and inversion algorithms applied to retrieve vegetation characteristics from different sensors. The radiative transfer models range from simple dimensional ones to sophisticated three dimensional models. Similarly, the inversion techniques vary from empirical-statistical techniques to machine learning and iterative optimization techniques. Such diversity in techniques and assumptions poses a number of challenges and difficulties in using and combining the products of these sensors. These products differ sometimes noticeably from each other even for the same area and same date.

1.2.5. Temporal considerations

Timely data is important for vegetation monitoring in environmental modeling. For instance, local scale agricultural applications demand high spatial and temporal resolution data at critical time steps over the growth period. While the other necessary factors for environmental models can be collected daily (like meteorological variables), the temporal resolution of available optical sensors does not allow for frequent updates of vegetation characteristics due to the revisit time of the sensors and cloud cover. Platforms acquiring optical data at high or intermediate spatial resolutions (1m–100m) have a nominal revisit frequency of about a few days to a few weeks, which becomes significantly lower because of clouds. Even coarse resolution optical satellites acquiring daily observations are prone to cloudiness which often hampers their effective use. To cope with this problem, vegetation products are often derived from a set of observations accumulated over a specified time period (e.g. 10 days for the VEGETATION LAI product). The temporal window over which the observations are accumulated differ from one sen-

sor to another. These different time intervals often introduce artificial variations in the products. Although, such variations may be smoothed out by some techniques, the degree of smoothness need to be carefully estimated (Quaife et al., 2008).

1.2.6. Uncertainty of the retrievals

In addition to the retrieved values of vegetation properties, it is important to have knowledge of uncertainties associated to these retrievals. An understanding of the source of the uncertainties can help in improving the quality of retrievals. Further, characterization of such uncertainties is a key factor in data assimilation and multi-sensor variable retrieval. Therefore, special attention has to be given to the development of techniques capable of estimating uncertainty accurately. Among the available vegetation products, the new generation of MODIS products are delivered with uncertainty on the retrieved variables, however, the other products do not provide such information.

1.3. Towards improved retrieval of vegetation variable

Limitations and shortcomings outlined in the previous sections are relevant to three factors on which the retrieval of vegetation variables is strongly dependent; (I) quality of the radiative transfer model used for forward simulation, (II) robustness of inversion technique and (III) quality of satellite observations (Jacquemoud et al., 2000; Meroni et al., 2004). To improve variable retrieval, attention has to be paid to the development of all these issues together. The limitations discussed in § 1.2.1 arise from the fact that the at-sensor radiance needs to be converted to TOC reflectance. A practical solution, as mentioned above, is to use a coupled soil–vegetation–atmosphere model instead. The four-stream approach (Verhoef and Bach, 2003b, 2007) addresses the need for TOA radiance simulation assuming a flat surface. The approach integrates the Soil-Leaf-Canopy radiative transfer model (SLC) with the atmospheric radiative transfer model MODTRAN. Four surface reflectance factors calculated by the SLC are coupled with atmospheric coefficients extracted from MODTRAN to simulate TOA radiance. The atmospheric coefficients are obtained from three MODTRAN runs at 0, 0.5 and 1 surface albedos with the assumption of Lambertian flat surface. Since direct call to the MODTRAN code is computationally intensive, particularly using its accurate mode, look-up-tables can be prebuilt and used for different atmospheric conditions. For rugged terrain, the four stream approach has to be modified to account for the topographic effects as mentioned in § 1.2.2.

The robustness of inversion depends on the inversion algorithm as well as the assumptions on the free and fixed variables as described in § 1.2.3. The sensitivity of output radiance to input variables can be analyzed to investigate the robustness of the model assumptions on the input variables during inversion. A global sensitivity analysis method capable of capturing the main influence of individual model inputs on the output radiance plus the mutual interaction effects between different inputs will help to identify influential and non-influential variables. This will also determine how robust the assumptions are. As available canopy variable retrieval methods are usually based on analyzing radiometric data from single-sensor often mono-directional and mono-temporal (Dorigo et al., 2007), a great potential lies in the combination of data from observations

with different angular, spectral, spatial, or temporal properties (Bacour et al., 2002; Verhoef, 2007; Schaepman et al., 2005). The synergy of a time series of optical satellite observations from a variety of sensors can be exploited to improve the retrieval of vegetation variables. Information from different sensors may assist in the variable estimation by limiting potential ambiguities. This involves observations at different spatial, spectral, temporal and angular resolutions, etc. The increase in the number of spectral and angular bands along with better temporal resolution would increase the dimensionality of data and hence helps to mitigate problems like ill-posedness. However, high dimensionality will also lead to more complicated data processing and the cost and time of computations increase with the size of data. Therefore, the use of robust and efficient retrieval approaches is inevitable in order to take full advantages of all available data. A multi-sensor approach applied to a temporal sequence of radiometric data acquired by different sensors can increase the frequency of usable observations, as well as improve spectral, spatial and angular sampling (Verhoef, 2007). This, in turn, improves mapping and monitoring of vegetation variables over time and allows having a unified product of multiple satellite images instead of a catalog of single satellite images. Even when no observations are available due to orbital configuration or cloudiness, the prior estimates are taken.

1.4. Scope and objectives

This research contributes to improving the retrieval of vegetation variables from optical satellite observations. The primary objective is to explore the potential of a multi-sensor approach in retrieving vegetation characteristics. The research hypothesis is that a generic multi-sensor approach capable of dealing with a diversity of optical sensors by integrating them together would allow for frequent updates of vegetation biophysical and biochemical products as well as it delivers better retrievals than single sensor. To achieve this objective, the following specific research questions are formulated:

- A. Can a sensitivity analysis be exploited to help determining model parameterization and assumptions prior to inversion?*
- B. Is a generic optical multi-sensor approach using TOA radiometric data to retrieve biophysical and biochemical vegetation variables feasible?*
- C. What are the advantages of a multi-sensor variable retrieval over a single sensor variable retrieval approach?*
- D. How significant are the topographic effects on TOA radiance in terms of variable retrieval?*

1.5. Outline

The core of this thesis is a series of papers addressing the aforementioned research questions and one chapter is devoted to the theoretical background on the remote sensing of vegetation.

Chapter 2 provides insight into the principles of remote sensing for vegetation analysis and modeling. The key elements of optical remote sensing over land will be described and details are given on different components of quantitative remote sensing of vegetation. Major variables driving the output radiance/reflectance from soil, leaf, canopy and atmosphere are identified and elaborated. A review of inversion algorithms for variable retrieval is given and various aspects of retrieval are discussed.

Chapter 3 investigates the use of sensitivity analysis to quantify the influence of different variables on the output radiance and reflectance. An improvement to the design and sampling of global sensitivity analysis is introduced for efficient sensitivity analysis of computationally expensive models with results comparable to sophisticated global methods. The sensitivity of TOA radiance and surface reflectance to input biophysical and biochemical variables are analyzed and compared. Influential and non-influential variables are identified and the interaction effects among input variables are discussed. Besides, the effect of solar/view direction on TOA radiances sensitivity to the input variables is also analyzed.

Chapter 4 provides a proof of concept for a multi-temporal, multi-sensor approach to retrieve vegetation variables using data collected by different imaging spectral-radiometers over time. This chapter presents an overview of the results and challenges in utilizing the multi-temporal, multi-sensor approach and the Bayesian inversion technique in the retrieval of terrestrial vegetation properties. Different aspects of the multi-sensor approach are discussed and the applicability of the Bayesian inversion technique is explored.

Chapter 5 addresses the generalization of TOA radiance simulation using the four stream approach to rugged terrain. The approach accounts for the topography-induced contributions from neighboring features into the field of view of the sensor. Moreover, a new formulation is proposed for the calculation of the atmospheric coefficients in which only two MODTRAN calls are required.

Finally, the thesis is concluded by Chapter 6, where the main results and findings from the core chapters are integrated and discussed. Suggesting directions for future research efforts ends the thesis.

2

Retrieval of vegetation properties

2.1. Remote sensing of vegetation

According to Goel (1988), optical remote sensing over vegetated surface may be modeled by considering the following subsystems: (I) the solar subsystem, as the main source of radiation defined by solar zenith and azimuth angles and spectral intensity; (II) the atmosphere, characterized by absorption and scattering of radiation mainly due to aerosols, water vapor and other gases; (III) the vegetation canopy, characterized by optical properties and architectural parameters; (IV) the background (e.g. soil), characterized by the optical properties of soil; and (V) the optical sensor, determined by sensor characteristics and observation geometry. The recorded at-sensor signal can, therefore, be expressed as a wavelength dependent function of the properties of all subsystems by modelling radiative transfer processes along the sun-target-sensor path. When electromagnetic radiation impinges on a surface, three different interactions occur; reflection, absorption and transmission. The optical properties of vegetation canopies depend on the density and orientation of canopy elements. The soil optical properties also contribute to the output reflection of the canopy especially for sparse vegetation cover. In the following sections, we first define key biophysical properties of vegetation, then describe radiative transfer processes and modelling approaches along the sun-target-sensor path. Different techniques to retrieve vegetation properties will be briefly reviewed along with their advantages and disadvantages and a discussion on the challenges and requirements for a multi-sensor retrieval approach will conclude the chapter.

2.2. Physical definitions

The optical properties of a soil-vegetation-atmosphere system depend on a large number of components (Verstraete et al., 1996), which do not equally influence the output reflectance/radiance or are equally important for land surface process models. There are a few variables that are essential as inputs to such models. Leaf area index (LAI), chlorophyll content and fractional of vegetation cover (fCover) are among the most important vegetation biophysical and biochemical properties for land surface models that can be derived from remote sensing observations. The retrieval of these three variables forms the focus of this thesis and they are briefly described below. LAI is the leaf area density vertically integrated across the canopy and is geometrically defined here as the total one-sided green leaf area for broadleaf canopies and the projected needle leaf area for coniferous canopies over ground surface area (Chen and Black, 1992; Myneni et al., 2002). LAI is a quantitative indicator of the amount of green foliage in the canopy which determines radiation regimes and the capacity of the vegetation for photosynthesis and water exchange in an ecosystem (Law et al., 2001). It determines the surface-atmosphere interaction and thus it has a key role in the exchange of different gases, mass and energy between the surface and the atmosphere (Knyazikhin and Martonchik, 1998).

LAI can be measured in situ directly (e.g. by destructive sampling or non-harvesting litter traps) or estimated indirectly (remotely) using different instruments (Weiss et al., 2004). Direct methods are often considered to be the most accurate measurements of LAI (Law et al., 2001), though they cannot be applied in many cases because of their destructive nature and also time and labor demand. Instead, indirect methods offer a faster, nondestructive and easier way to measure this property. Indirect methods are ba-

sically based on the measurement of gap fraction and light transmission through canopies. A variety of instruments have been developed to measure either gap fraction distribution (e.g. LAI-2000 Plant Canopy Analyzer (LI-COR, Lincoln, Nebraska USA)) or gap size distribution (hemispherical photography) to estimate LAI at point locations or over an area. When no correction for clumping and senescent leaves is applied, the measured variable corresponds to effective LAI rather than actual LAI (Baret et al., 2010). Even having applied such correction, due to the assumption of random foliage distribution, the clumping effect will be partially accounted for and the delivered variable is still effective LAI (Richter et al., 2011). This is also the case when applying physically-based model inversion where the retrieved LAI corresponds to allometric or effective estimates linked to the particular spatial resolution of the measurements (Pinty et al., 2004). In situ measurements (direct and indirect) are labor-demanding and time consuming and thus very expensive to accomplish. Therefore, it is not feasible to measure LAI in situ for regional and global scales due to its considerable variation in time and space. This makes the use of remote sensing a candidate approach to estimate LAI indirectly (Duveiller et al., 2011).

Another important canopy attribute is the fraction of green vegetation occupying an unit area of horizontal soil (fCover). It can be defined as the gap fraction at the nadir viewing angle. fCover determines the fraction of Absorbed Photosynthetically Active Radiation (fAPAR), though it is independent of illumination conditions (Jimenez-Munoz et al., 2006). Knowledge of fCover and LAI as the main canopy structure properties provides complementary information to describe the canopy radiation environment, microclimate and the three-dimensional structure of vegetation (Weiss et al., 2004). Furthermore, LAI and fCover long-term (e.g. seasonal) variations are vital observations for climate and drought monitoring. There exist different ground-based methods to measure fCover, however, likewise LAI such measurements are time consuming and tedious and often not practical over large areas. fCover has been less retrieved from remote sensing observations compared to LAI and chlorophyll content. This is due to the fact that widely used physical models for the retrieval of biophysical variables are limited to 1D radiative transfer, representing a vegetation canopy as a turbid medium. In the turbid medium assumption the canopy is assumed to be homogeneous, i.e. fCover= 1. This is certainly problematic in case of sparse to medium vegetation cover. It is therefore more efficient and advantageous to retrieve LAI and fCover together.

Photosynthesis is the process that absorbs light energy, converts it to chemical energy and converts water and dioxide carbon into oxygen and organic matter. The capacity of vegetation for photosynthesis is mainly driven by the chlorophyll concentration of leaves. Leaf chlorophyll content strongly affects reflection in the visible part of the spectrum ($0.4 - 0.7\mu m$) and therefore can be estimated by satellite observations having spectral bands in this region of the spectrum. Chlorophyll content is usually measured in micrograms per square centimeter of leaf disc ($\mu g/cm^2$). As pointed out earlier (similar to LAI and fCover), direct in situ measurements of chlorophyll poses a number of limitations which makes the use of remote sensing beneficial in estimating this property. A more detailed discussion on the leaf spectral behavior related to leaf chlorophyll content is given in Section 2.3.2.

2.3. Radiative transfer modeling

Radiative transfer (RT) models simulating the spectral reflectance/radiance of the soil-vegetation-atmosphere system are frequently used to retrieve biophysical properties of the Earth's surface and the atmosphere by model inversion. The radiative transfer describes the change (i.e. loss and gain) in specific intensity of radiation I_ν because of extinction and emission while propagating through a medium:

$$dI_\nu(x, \nu, \theta) = -\kappa(x, \nu) I_\nu ds + j(x, \nu, \theta) ds \quad (2.1)$$

where κ is the volume extinction coefficient and j is the emission coefficient for photons traveling a distance s in a specific direction at a given position x in a medium. Defining $\mu = \cos(\theta)$, and optical depth as $\tau(\nu) = \int_0^x \kappa(x, \nu) dx$, we can rewrite the radiative transfer equation;

$$\mu \frac{dI_\nu}{d\tau} = I_\nu - S_\nu \quad (2.2)$$

where $S_\nu = j(\nu)/\kappa(\nu)$ is the source function. Exact analytical solutions of the radiative transfer equation can only be obtained for simplified situations (e.g. no scattering). If there is no scattering, for I at given κ at surface of plane-parallel slab with optical depth τ_1 ;

$$I_\nu = I_\nu(\tau_1) \exp(-\tau_1) + \int_0^{\tau_1} S_\nu(t) \exp(-\tau_1) dt \quad (2.3)$$

If S is known the integral will be straightforward, however in most cases S is dependent on I and the integral equation must be solved first. There is a number of approximate analytical solutions of the radiative transfer equation. Assuming a homogeneous medium with boundary layers and single scattering particles is one of such approximate solutions. However, in realistic situations (e.g. multiple scattering) where an accurate solution of the equation is needed, numerical solutions must be used to solve the radiative transfer equation. We will further discuss different solutions to the equation in case of vegetation canopies in detail in Section 2.3.3.

The Soil-Leaf-Canopy (SLC) RT model (Verhoef and Bach, 2003b) is an analytical radiative transfer model coupled with the atmospheric RT model MODTRAN used to simulate top of atmosphere radiance and reflectance. The SLC calculates surface reflectance factors and consists of a soil BRDF model (modified Hapke (1981) model), a leaf radiative transfer model (PROSPECT) and a canopy radiative transfer model (4SAIL2). The SLC follows a bottom-up approach to simulate top of canopy reflectance implementing RT models of soil, leaf and canopy and it is described in this section. The optical properties of the influential variables in each medium will also be discussed.

2.3.1. Soil level

Soil is a major part of the Earth's surface observed by remote sensing and it contributes significantly to the output reflectance of a vegetation canopy. This contribution is more significant when the vegetation cover is sparse and the background soil is exposed to the sensor, especially for nadir viewing and in the hot spot direction. Therefore, a better

conceptual understanding of soil optical properties is necessary for quantitative signal modeling and retrieval. The optical properties of soil are a complex function of the soil main physical and chemical properties such as soil moisture content, surface roughness, mineral and organic composition.

Soil mineral grains of different sizes and shapes absorb solar radiation causing lower reflectance, mostly in the middle infrared, depending on their chemical compositions like carbonates, sulfates and clay minerals (Anderson and Croft, 2009). Organic matter influences the chemical and physical properties of soil and mainly affects soil reflectance indirectly due to the variation in the structure and water retention capacity of soil. The overall soil reflectance decreases with the increase of soil organic matter over the entire spectral range from 400 nm to 2500nm (Palacios-Orueta and Ustin, 1998). Iron oxide minerals color the soil red or brown due to hematite or goethite respectively. The soil iron oxide content shows generally a negative correlation with the organic matter content (Palacios-Orueta and Ustin, 1998). The iron oxide content modifies soil reflectance at shorter wavelengths (less than 1100 nm). Strong absorption in the soil spectra occurs around 900 nm due to iron oxide content. Soil surface roughness is another important factor due to the shadowing effects of soil aggregates. In general, the rougher the soil, the lower the reflectance is (Walthall et al., 1985). The soil moisture observable by optical remote sensing is approximately the moisture content within a very thin layer at the soil surface (Anderson and Croft, 2009). Soil moisture has a significant impact on the soil spectra over the entire range of the spectrum. Figure 2.1 illustrates the soil moisture impact on the soil spectra. The effect of soil moisture is stronger in the infrared part (middle infrared and SWIR) of the spectrum.

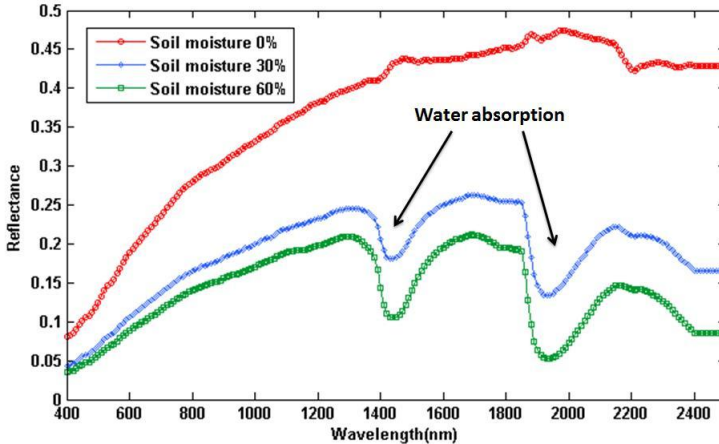


Figure 2.1: Soil moisture impact on a typical soil reflectance from 400nm to 2500nm

The soil spectral reflectance is known to be less variable compared to the typical vegetation spectra where it regularly increases with wavelength forming a convex curve in general. Liang (2004) has grouped approaches for soil reflectance modelling into three major categories; approximate, numerical and geometrical-optical. The Hapke's soil model (Hapke, 1981, 1984; Hapke and Wells, 1981) is a widely used model to simulate soil

reflectance in the category of approximate solutions. The soil BRDF is highly anisotropic even more than most vegetated surfaces (Goel, 1988), though it is often assumed to be a pure Lambertian diffuse reflector characterized by a hemispherical reflectance in most canopy reflectance models. However, this assumption may lead to serious deviations from actual soil bidirectional reflectance measurements. A non-Lambertian extended version of the Hapke's BRDF soil model containing the hotspot and soil moisture effects has been applied to calculate soil reflectance and its variability with moisture (Verhoef and Bach, 2007). The model is a semi-empirical model which assumes the soil as a semi-infinite medium and scattering inside the soil medium is described by a scattering phase function which is parameterized as a second-order Legendre polynomial (Pinty et al., 1989). It also contains a hot spot correction factor in the single scattering contribution to the computed bi-directional reflectance. The model requires five input parameters: phase function parameters b and c , hot spot (half) width parameter h , hot spot magnitude parameter $B0$ and soil moisture percentage. The hot spot parameters ($B0$ and h) and phase function parameter c only affect the bi-directional reflectance while phase function parameter b has an influence on all the reflectance factors (Verhoef and Bach, 2007).

2.3.2. Leaf level

Leaves perform photosynthesis by absorbing sun light and carbon dioxide. The sun light is converted into chemical energy and is stored as carbohydrates. Leaves can also store nutrients and collect water. Figure 2.2 depicts a leaf cross section. The outer surface of the leaf is called epidermis, where pairs of cells build a gateway in the lower epidermis for gases including oxygen, carbon dioxide and water to flow in and out. The palisade layer is located beneath the upper epidermis layer. Chloroplasts which contain chlorophyll are located in the palisade layer, and therefore most of the leaf photosynthesis occurs in this layer. The spongy layer below the palisade layer includes loosely packed spongy mesophyll cells to allow gas exchange through the leaf.

Leaf spectral behavior is determined by its chemical and structural properties (Jacquemoud and Baret, 1990). The main properties characterizing leaf spectral response are leaf pigment content (such as chlorophylls and carotenoids), leaf tissue structure (determining the size of aerial interspaces between cells), and the structure of the leaf surface (e.g., waxes and hairs). The spectral reflectance of leaves from $0.4\mu\text{m}$ to $2.5\mu\text{m}$ can be subdivided into three regions, visible ($0.4 - 0.7\mu\text{m}$), near infrared NIR ($0.7 - 1.3\mu\text{m}$) and middle-infrared ($1.3 - 2.5\mu\text{m}$).

The leaf pigments control the radiation regime of leaves in the visible domain by strong absorption of light, resulting in lower reflectance of leaves in this domain (Ustin et al., 2009). Among leaf pigments, chlorophyll (a and b) are the main absorbers of radiation in which they can absorb up to 70%-90% of the incident solar radiation (Campbell, 1986). Chlorophyll gives leaves their green color by absorbing red ($\sim 670\text{ nm}$) and blue ($\sim 500\text{ nm}$) spectral wavelengths as a result of electronic transitions in its molecular structure. Chlorophyll only influences the visible spectrum and is transparent to infrared radiation. The absorption in the infrared region is restricted to the dry matter compounds such as cellulose, lignin and other structural carbohydrates. Instead, leaf tissue structure explains the main optical properties in the near infrared part. The high reflectance

of leaves in the infrared is mainly due to the spongy mesophyll cells placed in the back or interior of a leaf. The number of intercellular air spaces in the lower mesophyll layer is the main factor responsible for the scattering. Strong absorption by leaf water content characterizes the middle infrared region with absorption bands centered at 1450 nm and 1950 nm.

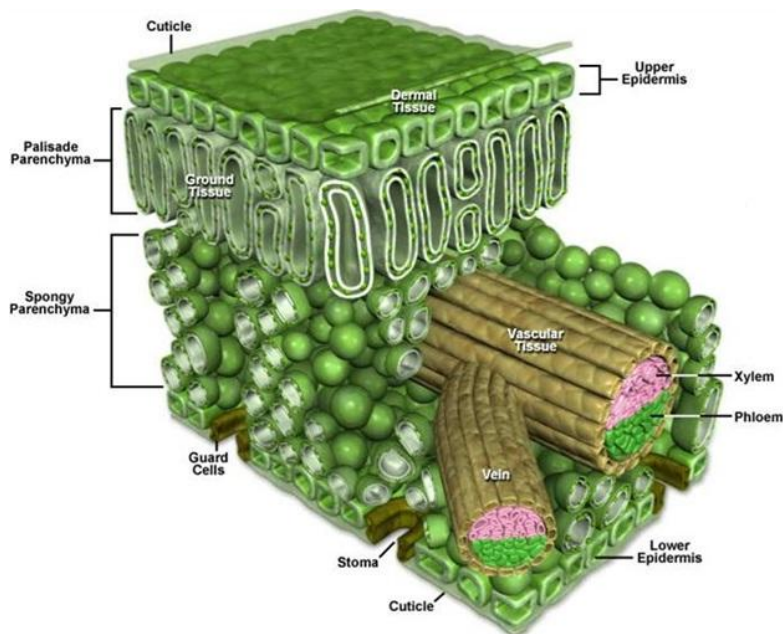


Figure 2.2: Leaf cross section (image courtesy <http://www.bladmineerders.be>)

A number of radiative transfer models such as the generalized “plate model” (Allen et al., 1970), PROSPECT (Jacquemoud and Baret, 1990), the conifer leaf model LIBERTY (Dawson et al., 1998), LEAFMOD (Ganapol et al., 1998) and SLOP (Maier et al., 1999) have been developed to calculate leaf optical properties. Among them, the PROSPECT model has been extensively used and well validated in calculating specific absorption and scattering coefficients of leaf properties (Fourty et al., 1996; Jacquemoud et al., 2009). The PROSPECT simulates leaf reflectance and transmittance as a function of leaf biochemical content and leaf anatomical structure. The inputs are the leaf chlorophyll concentration, dry matter content, equivalent water thickness, and the leaf internal structure parameter (leaf thickness). A modified version of the PROSPECT is used in this study that includes also the concentration in senescent material of leaf (Verhoef and Bach, 2003b). The model provides the leaf directional-hemispherical reflectance and transmittance factors as output.

2.3.3. Canopy level

A vegetation canopy is quite a complicated system that consists of many components: branches, stems, leaves, stalks, bark, flowers, etc. These components have different

optical properties and are distributed and oriented in a complex manner. Canopy reflectance is, therefore, the result of the electromagnetic radiation interacting with such components and the background (e.g. soil) (Goel, 1988). However, the leaf-related factors are the key factors dominating canopy spectral reflectance. Accordingly, we only consider leaf-related factors in a canopy to calculate canopy spectral reflectance. The reason to ignore the optical properties of the other vegetation components, like the woody parts of branches, stems and trunks is twofold. This is, first, due to the fact that canopy reflectance models do not often model the spectral behavior of these components and, second, because of the limited influence of such components on canopy spectral reflectance as the leaves are the main light intercepting plant organs (Bousquet et al., 2005). Leaves vary in shape, size and orientation and they are not distributed evenly within the canopy. This implies that apart from the biochemical properties of leaves, information on the amount, orientation and distribution of leaves within the canopy is required to model the canopy reflectance. Leaves intercept radiation by scattering and absorption which means the larger the number and area of leaves, the lower the canopy transmittance is. The probability of photons to penetrate deeper into the canopy without being absorbed or scattered is not only dependent on the number of leaves but also on the gap fraction of the canopy. This gap fraction is determined by the non-uniform distribution of leaves. The so-called clumping effect explains this gap fraction and it is important to model this effect in a canopy. Another important factor is the leaves angular distribution that is described by the Leaf Inclination Distribution Functions (LIDF). More detail on the canopy biophysical and structural variables will be given in the following chapters.

Canopy reflectance modeling was primarily introduced in the early 1950s, to describe the radiation regime within vegetation canopies (Goel, 1988). Further development followed with the advent of satellite observations in order to extract desirable information on the status and conditions of vegetation from remotely sensed data ((Roberts, 2001). The first canopy reflectance model was developed by Monsi and Saeki (1954) and since then several models have been proposed to describe the radiation regime within a vegetation canopy and to simulate canopy reflectance. They can all be grouped into four categories; Turbid medium, Geometrical-Optical, Hybrid models and Computer simulation (Liang, 2004; Roberts, 2001). These models are well-reviewed in the literature (Goel, 1988; Liang, 2004; Casa, 2003). It is beyond the scope of this study to go into details of these models and the readers are referred to works cited above. Here we will only briefly describe each category and give more insight into the turbid medium theory since it is the basis for the radiative transfer model used in this study (i.e. SLC).

Turbid medium models are based on the theory developed by Kubelka and Munk (1931) which models radiation propagation in one dimension for a parallel-plane medium. The theory uses two monochromatic downward and upward fluxes to explain the diffuse light flux (Goel, 1988). In this theory, the canopy is described as a series of plane parallel horizontal slabs composed of small absorbing and scattering elements with given optical properties. These small elements are randomly distributed within the canopy and oriented in given directions and the variation of diffuse fluxes is modeled by absorption and scattering coefficients of such elements. The location of such elements is not determined and the canopy architecture is described by a statistical distribution

of the orientation of these elements (Liang, 2004). A set of equations derived from the diffuse fluxes are used to approximate the radiative transfer equation in this case. This assumption best fits homogeneous vegetation (e.g. dense crops), but for row crops and sparse vegetation the assumption does not hold. Turbid medium models are mathematically simple and hence computationally efficient. These properties have made turbid medium models of interest for canopy reflectance modeling and variable retrieval.

Geometrical-Optical models (Li and Strahler, 1986) treat the canopy as a distribution of geometric objects, such as cylinders and cones, with known optical properties placed on a flat surface. The radiation interception and shadowing by these geometric shapes and reflectance from the background surface determine the canopy reflectance. These models can describe sparse vegetation such as planted trees and shrublands.

The Hybrid models combine turbid medium with geometrical-optical models. The spatial heterogeneity of geometrical-optical models with the realistic radiative transfer behavior of turbid medium models are integrated to better model the radiation propagation within a canopy volume. The canopy is described as a series of sub-canopies (e.g. geometric shapes) which are individually treated like a turbid medium. This allows the modelling of gap probabilities and distributions along with single and multiple scattering (Vuolo, 2007). However, the complexity of the hybrid models makes them computationally intensive and as a result less practical in canopy reflectance simulation.

Computer simulation models allow for more realistic simulation of the canopy reflectance, where the canopy is treated as a three-dimensional space composed of individual vegetation elements distributed within the canopy. The typical methods to describe the radiation propagation within a canopy are Monte Carlo methods (e.g., (Lewis and Muller, 1993; Govaerts, 1996)) and radiosity techniques (e.g., (Borel et al., 1991)).

There is a large number of canopy reflectance models available in all four categories mentioned above and their performance has been compared in the RAMI project (Widlowski et al., 2007). Numerical models based on computer simulation (e.g. ray tracing) can simulate canopy reflectance more accurately, but they are computationally demanding and hence have a very limited use in variable retrieval. Analytical radiative transfer models are often computationally affordable and offer suitable alternatives.

The analytical radiative transfer model 4SAIL2 (Verhoef and Bach, 2007) is used to simulate canopy reflectance in this study. The model is the most recent version of the Scattering by Arbitrarily Inclined Leaves (SAIL) radiative transfer model proposed by Verhoef (1984). The SAIL model is, in turn, an extension of the Suits model which was the first turbid medium model developed by Suits (1973). In the Suits model, leaves are assumed to be tiny flat Lambertian scatterers that are randomly distributed within the canopy where the leaves are replaced by their horizontal and vertical projections. The soil is also treated as a Lambertian reflector. The model considers only downward and upward diffuse radiation fluxes and only vertical and horizontal leaves. The SAIL model allows any distribution of leaf angle. The first SAIL model was not able to model the hot spot effect due to the assumption of an infinite number of non-dimensional Lambertian scatterers. This shortcoming was rectified in the later versions of the SAIL model. Most

canopy reflectance models only consider green leaves, but a canopy is not only composed of green leaves, but also brown leaves. The clumping effect, as noted above, is another key factor that is often not taken into account in many canopy reflectance models. The 4SAIL2, the most recent member of the SAIL family, is a hybrid model capable of taking into account two leaves layers (green and brown) and the clumping effect is also modeled by two parameters: tree shape factor (Zeta) and the vertical crown cover (Cv). The 4SAIL2 treats the soil as a non-Lambertian reflector and accounts for soil moisture as well. The detailed explanation about 4SAIL2 and SLC are given in the relevant sections in the following chapters, therefore we avoid excessive detail here.

2.3.4. Atmosphere level

The earth's atmosphere is composed of a complicated mixture of various gases, molecular and aerosol particles with different sizes and sources that are spatially and temporally distributed. The atmosphere has a complex impact on the radiance observed by satellites. This impact is particularly considerable on the visible and infrared radiation. The atmosphere influences the radiation twice, on the downwelling radiation from the sun and on the upwelling reflected radiation from the surface. Absorption and scattering effects are the two major atmospheric effects on the solar radiation. The absorption effect results in a loss of the intensity of the radiation reflected from the surface and therefore reducing the contrast of the surface. The scattering process modifies the propagation direction and increases the radiation reaching the sensor. Scattering determines diffuse radiation in the atmosphere.

Water vapor, carbon dioxide, ozone, oxygen, methane and carbon monoxide are mainly responsible for the gaseous absorption in the solar spectrum. To correct radiometric measurements by multispectral sensors, more attention is paid to the first three since their concentration and vertical distribution is variable in space and time. The concentration of such gases in the atmosphere, except water vapor, varies slowly in both space and time. Because of their low variability and minor effects on radiation, it is reasonable to use default value determined from climatology data (Guanter, 2006). On the contrary, water vapor has a very high variability and plays a crucial radiative role (Rahman et al., 1993a). This makes water vapor a very important factor that has some absorption bands in the visible and near-infrared regions and needs to be precisely considered.

Molecular scattering in the atmosphere can be described by Rayleigh scattering (Kaufman, 1984). Therefore, the contribution of the gaseous scattering on the radiation is adequately modeled (Guanter, 2006). In contrast, atmospheric aerosols are composed of various particles with different sizes, shapes, chemical and physical properties that are heterogeneously distributed in time and space. Consequently, aerosols modeling remains a cumbersome and challenging task in atmospheric modeling and correction (Guanter, 2006). When the concentrations of different gases and aerosols are known, the optical properties of the atmosphere can be modeled by an accurate radiative transfer code. This requires a rather detailed knowledge of the state and composition of the atmosphere at the time of the image acquisition. This knowledge may come from ancillary data on atmospheric state and composition taken from standard atmospheric profiles, or a more logical alternative is to retrieve them simultaneously from the remote sensing data itself (Rahman et al., 1993b). This alternative can be performed using sensor spec-

tral bands located in the spectral regions sensitive to those atmospheric parameters.

The radiative transfer equations are well-known in the atmospheric research field and several radiative transfer codes have been already reported in the literature to model radiation transfer in the atmosphere (Goody and Yung, 1989). The most frequently used atmospheric radiative transfer codes in remote sensing are the MODerate resolution atmospheric TRANsmittance and radiance code (MODTRAN) (Berk et al., 1987) and Second Simulation of the Satellite Signal in the Solar Spectrum (6S) (Vermote et al., 1997). The 6S code is based on the successive orders of scattering approximations and is known to be computationally fast with reasonable accuracy to simulate at-sensor reflectance and radiance for lambertian and anisotropic surfaces. The code has been implemented in generating lookup tables in the MODIS atmospheric correction procedure (Vermote et al., 2002). MODTRAN is developed initially from the LOW resolution TRANsmittance 7 (LOWTRAN 7) model. The code represents the state-of-the-art radiative transfer code and models the scattering and the absorption effects of the atmospheric processes precisely with high spectral resolution up to 1cm^{-1} . The scaled DISORT (DIScrete Ordinate Radiative Transfer) algorithm is integrated for accurate computations of atmospheric multiple scattering and the correlated k algorithm is applied for the spectral regions with significant absorption effects. Regarding the absorption band model, the HITRAN96 database is used in two modes of very accurate 1cm^{-1} band model and an optimized 15cm^{-1} model for the cases that high spectral resolution is not needed. MODTRAN is highly flexible in the input parameters, since both user-defined and predefined profiles for different scenarios are accepted. MODTRAN also includes the surface BRDF where a BRDF model may be chosen from a list of available models or may be defined by the user. All these features make MODTRAN a good candidate for realistic simulation of at-sensor radiance (Guanter and Kaufmann, 2009; Laurent et al., 2011a; Schlapfer and Nieke, 2005; Verhoef and Bach, 2007, 2012) and for atmospheric correction (Adler et al., 1999; Schlapfer and Richter, 2002) from the ultraviolet to the thermal infrared wavelengths. MODTRAN provides more accurate results at a higher computational cost than the 6S code. However, as reported in the literature, the difference in simulating at-sensor signal between the two codes can reach up to 10%, in particular for absorptions above 2000nm (Schlapfer et al., 1998). Consequently, MODTRAN is preferable for narrow band hyperspectral data.

2.3.5. Coupled surface-atmosphere RT model

At-sensor spectral radiance is the integrated sum of surface reflectance, atmospheric effects and target surroundings convolved with the sensor spectral and spatial response functions. To simulate at-sensor radiance, a surface RT model has to be coupled with an atmospheric RT model. This coupled modelling scheme has already been applied with success to simulate at-sensor radiance and reflectance by a number of authors (Fourty and Baret, 1997; Guanter and Kaufmann, 2009; Isaacs and Vogelmann, 1988; Laurent et al., 2011b; Rahman et al., 1993b; Schott, 2007; Verhoef and Bach, 2003b, 2007, 2012; Zhang et al., 2010). The four-stream theory (Verhoef and Bach, 2003b, 2007, 2012) can effectively model this integration with computational efficiency and accuracy. The four considered fluxes are two direct solar and observed fluxes and two downward and upward diffuse fluxes. The approach combines four surface reflectance factors calcu-

lated by SLC with six atmospheric coefficients extracted from MODTRAN. The approach has been validated against both synthetic data and satellite measurements (Verhoef and Bach, 2007; Widlowski et al., 2007). The comprehensive description of the four stream approach is given in the following chapters.

2.4. Retrieval of vegetation properties

Vegetation variable retrieval from satellite observations has quite a long history. Over the last decades, considerable effort has been devoted to developing techniques for the retrieval of vegetation properties. Detailed reviews of the existing retrieval techniques can be found in Goel (1989), Kimes (2000), Liang (2004) and Baret and Buis (2008). Retrieval techniques have been conventionally divided into two groups of empirical-statistical and physically-based techniques. A more appropriate classification of retrieval techniques has been proposed by Baret and Buis (2008) based on whether the focus is on the variable to be retrieved (variable-driven) or on the radiometric data used (radiometric data-driven) (Baret and Buis, 2008).

2.4.1. Variable-driven retrieval

In a variable-driven approach, a model is trained over a training dataset and the variable of interest is retrieved by finding the best match between the observations and the training data. The basic assumption is that remote sensing observables are directly related to the desired information about vegetation and the relationship can be described by spectral information from one spectral band or some algebraic combination of different bands (Verstraete, 1994). A typical approach is to apply a regression model linking vegetation indices to the variable of interest. This approach is fast, simple and easy to implement to obtain useful information from satellite observations. However, it presents a number of limitations and drawbacks. Most vegetation indices reduce the dimensionality of the dataset by combining information in two or a few spectral bands into an index (one dimension). They are influenced by a number of unwanted factors such as illumination and viewing geometry, background soil, atmospheric and topographic effects etc. It is not practical to design a vegetation index that is only sensitive to the variable of interest and insensitive to others. Moreover, vegetation indices require reliable ground truth data to be calibrated and often saturate and become insensitive to variation of the variable of interest. As a result, the use of regression-based retrieval techniques based on vegetation indices is restricted to the condition, time, site and sensor to which they have been calibrated.

Several other variable-driven techniques have recently been proposed such as Gaussian process (Verrelst et al., 2013b), support vector machines (Durbha et al., 2007), Artificial Neural Network (ANN) and Projection Pursuit (Duveiller et al., 2011). ANN techniques have also been gaining more popularity recently due to their computational efficiency and the capability of handling multivariate problems (Bacour et al., 2006; Baret et al., 2007; Duveiller et al., 2011; Fang and Liang, 2005; Liang, 2004; Schlerf and Atzberger, 2006). In these techniques, the learning data set is generated based on either experimental data or a model of radiative transfer. However, similar to the regression-based retrieval based on vegetation indices, variable-driven techniques often lack the funda-

mental physical basis and are limited to use in conditions over what they have been trained and calibrated (Verstraete et al., 1996).

2.4.2. Radiometric data-driven retrieval

In a radiometric data-driven approach, the objective is to obtain the estimate that minimizes the residuals between measured and modeled radiometric data. In this case, the calibration and training steps are not required. Radiometric data-driven approaches are based on the inversion of physically-based models and therefore there exists a physical understanding of the interactions between different variables and the radiation. However, the performance of such an approach is influenced by the level of ill-posedness of the inverse problem and the minimization algorithm used (Baret and Buis, 2008). Moreover, since physically-based models have to address the entire radiative transfer problem, they often require a large number of variables. This implies that the retrieval performance needs sufficient spectral and angular sampling of the surface BRDF (Kimes, 2000). A typical radiometric data-driven approach consists of four main components; satellite measurements, a physically-based model, an optimization (minimization) algorithm and an objective function (merit function). During model inversion, the optimization algorithm iteratively changes the free variables until the simulated spectral signature closely resembles the measured spectral and angular signature. The objective function provides a numerical measure of the resemblance between the measured and simulated signatures. Many optimization techniques have been used for implementing radiometric data-driven approaches including iterative optimization methods (Bicheron and Leroy, 1999; Jacquemoud et al., 2000; Laurent et al., 2013; Vuolo et al., 2008), genetic algorithms (Fang et al., 2003), look up tables (Hedley et al., 2009; Laurent et al., 2011b) and Monte Carlo Markov Chains (Zhang et al., 2005). Among them iterative optimization techniques and look up tables have been the most widely used in the literature (Baret and Buis, 2008). We first discuss the ill-posedness and then the three aforementioned popular techniques from both categories will be briefly explained.

2.4.3. Ill-posed problem

Remote sensing retrieval is by nature an ill-posed problem (Kimes, 2000). This is due to uncertainty in satellite measurements and model simulations and also due to the fact that the number of free parameters is often larger than the number of independent measurements. Hadamard (1932) formulated a problem to be well-posed if and only if the solution (i) exists, (ii) is unique and (iii) is stable over the solution space. If any of these conditions is violated, the problem is ill-posed. In an inversion practice, one or more of these conditions might not hold. For instance, it is well understood that biophysical variables may compensate for each other effect on spectral radiance, i.e. different combinations of variables can generate identical or very similar spectra (violating the uniqueness condition) (D'Urso et al., 2009). It is generally possible to mitigate the ill-posedness of the retrieval problem by imposing additional constraints that bias the solution which is called *regularization*. Different regularizations can be applied to stabilize the retrieval problem. Imposing spatial constraints (Atzberger, 2004), narrowing the solution space (Dorigo et al., 2007), decreasing the number of free variables (Baret and Buis, 2008), incorporating prior information into the retrieval (Combal et al., 2002) and

imposing temporal constraints (Lauvernet et al., 2008) are examples of solutions to alleviate the ill-posedness. One or more solutions may be applied in an inversion to cope with ill-posedness.

2

2.4.4. Optimization techniques

There is no particular optimization technique that can be applied efficiently to all sorts of retrieval problems due to the diversity of retrieval problems in different aspects. The choice of a technique for any particular case depends primarily on the properties of the cost function, the constraints as well as the number of free variables. There are a variety of techniques applied to retrieve land surface properties from satellite observations. Among all applied techniques, as noted above, three classes have been receiving most attention in the literature; iterative optimization, look up tables and machine learning techniques. We hereafter briefly review these techniques and discuss particularly advantages and disadvantages of different techniques.

2.4.4.1. Iterative optimization techniques

Iterative optimization techniques have been frequently employed to solve inversion problems in remote sensing (Baret and Buis, 2008; Goel, 1988; Kimes, 2000). The downhill simplex method (Nelder and Mead, 1965), the quasi-Newton method and the conjugate direction set method are among commonly applied iterative routines in remote sensing problems (Kimes, 2000). The iterative techniques are very flexible to incorporate different auxiliary information and can easily be adapted to new conditions. In addition, the iterative techniques give a clear understanding of the physical processes that take place as well as it is clear what is happening during inversion (Press et al., 2007). An iterative technique requires an initial guess which is arbitrary and it should only be within the feasible range of variables. The method refines the initial guess successively until convergence is reached with respect to some criteria. An objective function provides the numerical measure of similarity between the observations and simulations. Different weights can be attached to both the observations and variables to bias the search in favor of imposing specific conditions on the retrieval. In a typical remote sensing variable retrieval, the objective function compares the simulated spectral signature of an initial guess (solution) with the observed spectral signature. If the criteria are met, the initial solution is taken as the optimal solution, otherwise a new solution is explored. The step size and search direction to explore new solutions are iteratively optimized with respect to the increase (or decrease) in the objective function. Iterative techniques often require intensive computational resources and convergence is not guaranteed particularly if measurements are incomplete and noisy. These limitations can be partially overcome by careful model parameterization and by incorporating prior information into the retrieval as in the case of multi-sensor retrieval. However, this still remains an obstacle to the application of these techniques, particularly for high dimensionality retrieval problems where either the number of free variables or the number of observations is very large.

2.4.4.2. Look-Up-Table (LUT)

Look-Up-Tables (LUT) are easy to implement and yet capable of finding an approximate global minimum of the cost function fast. The procedure is straightforward in which

pre-calculated tables are generated for a number of simulated canopies by a radiative transfer model before the inversion. The Tables contain values (radiance/reflectance) that are indexed according to the canopy input variables. Then the best estimate that minimizes the given cost function is found by searching the pre-built tables instead of a direct call to the radiative transfer model. LUT has been frequently used in retrieving biophysical vegetation properties from remotely sensed data because of its simplicity and speed (Baret and Buis, 2008; Kimes, 2000; Liang, 2004). The primary advantage of LUT technique is its speed so that once the LUTs are constructed, the inversion is fast. This is because retrieving a value from the stored LUTs is often faster than performing the radiance simulation computation directly with a RT model. Another benefit is that convergence is guaranteed in these techniques since the search is done over all the pre-calculated values. A major short-coming of LUT techniques is its memory usage which is dependent on the size of the LUT. A further drawback is the challenge of efficient sampling of the variable space (e.g. canopy realizations) in terms of number and step size. The LUT size will exponentially increase when adding more levels in the variable space. The accuracy achieved in this way is directly dependent on the number of levels and the number of realizations used for generating the LUTs. Furthermore, any change to the conditions (e.g. different sensor) for which the LUTs are built, would require recalculation of the LUTs, which is considered a further limitation of these techniques.

2.4.4.3. Machine learning techniques

Machine learning optimization techniques are inspired by processes observed in the natural systems, such as human nervous system and animal colonies. They are a class of approximate methods that find an optimal solution based on known properties learned from the training dataset. Such algorithms have to be first trained over a sample training dataset, either empirical or synthetic. The model establishes some relationships (weights/coefficients) between the variables of interest and the observations based upon the training dataset, and then these coefficients are used to retrieve the required variables. There are a number of machine learning algorithms applied in biophysical variable retrieval over the past decades (e.g. (Atzberger, 2004; Bacour et al., 2006; Duveiller et al., 2011; Fang and Liang, 2005; Verger et al., 2011; Verrelst et al., 2012)). Machine learning methods are often fast to retrieve biophysical variables and once they are trained the retrieval is considerably fast. However, these methods present a number of drawbacks. The main criticism is about the “*black box*” nature of such methods in which there is no clear comprehension of the physical processes. Another issue is related to the selection of the training dataset. Another criticism is about the modification of the models, variables and parameters in the machine learning methods. This implies that the system has to be redesigned if any modification is made (e.g. number of spectral bands, number of inputs, illumination geometry, etc.).

2.5. Challenges and requirements in a multi-sensor variable retrieval

A multi-sensor variable retrieval approach is designed to integrate over time a variety of sensors with different spectral, spatial, angular and temporal properties. The in-

tegration brings together sensors with different characteristics (e.g. variable illumination/observation geometries) plus a large number of spectral bands. This poses a number of challenges into the retrieval problem such as high dimensionality and varying conditions from one sensor to another. These challenges limit the use of statistical retrieval methods such as machine learning methods as well as LUT based retrieval. The practicality of the machine learning methods is limited due to the requirement of reliable and intensive ground truth data to calibrate and train the algorithms. Therefore, the application of them is limited outside their training condition. Moreover, even in the same conditions, any change in the inputs/outputs would require training the model again. The usefulness of LUT based methods is also limited due to the dimensionality of the problem which requires considerably large LUTs. Therefore, the iterative optimization methods re-emerge as a feasible alternative for a multi-sensor approach. An appropriate inversion method for a multi-sensor retrieval approach has also to be capable of incorporating prior information and taking into account model, observations and variables uncertainties. Among different iterative techniques, the Bayesian model inversion offers a powerful framework for variable retrieval and uncertainty estimation. It allows the incorporation of prior information about the solution into the retrieval and it can also estimate the uncertainty of the retrieved variables. These features make the Bayesian model inversion a promising way for variable retrieval in the multi-sensor framework.

3

Global sensitivity analysis of the spectral radiance of a soil-vegetation system

Abstract: We analyzed the sensitivity of Top-Of-Atmosphere (TOA) radiance and surface reflectance of a soil-vegetation system to input biophysical and biochemical parameters using the coupled Soil-Leaf-Canopy radiative transfer model SLC and MODTRAN. We applied variance-based global sensitivity analysis for different atmospheric conditions and observation configurations. Among 23 input parameters, crown coverage, leaf area index, leaf inclination distribution function and soil moisture were found to be the most influential parameters driving the output variance of the radiance between 400 and 2500 nm with a few exceptions. Hapke's soil parameters and the canopy layer dissociation factor were recognized to have marginal influence on the output radiance. It is also found that a large portion of uncertainty in the output radiance is driven by the interaction effects among input parameters in the visible ($\sim 550nm$), whereas the red-near infrared ($\sim 670nm$), seems to have fewer interaction effects. The effect of solar/view direction is found to be significant on TOA radiance sensitivity to the input parameters. The results also confirmed that the sensitivities of surface reflectance are comparable to the TOA radiance sensitivities when the atmosphere is clear and visibility is high. Since coupled surface-atmosphere RT models can be computationally intensive, this work also introduces an improvement to the design and sampling of screening methods for efficient sensitivity analysis of computationally expensive models. The improvement is based on three elements: a) generating sample points by Sobol's se-

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quence generator; b) variational analysis in the parameter space using the winding stairs method; c) use of mean and variance sensitivity measures. The results with 1200 model runs demonstrated high correlation (92%) with variance-based global sensitivity analysis using 49,152 model runs, in determining the most influential and non-influential parameters.

3.1. Introduction

Terrestrial targets are characterized by heterogeneity at all scales and the observed spectral radiance across the $0.4\mu\text{m}$ – $2.5\mu\text{m}$ spectral region is determined by a complex combination of target geometry and bio-geophysical and chemical composition of target elements (Jacquemoud and Baret, 1990; Verstraete et al., 1996). Extraction of information on observed targets from measurements of spectral radiance becomes significantly more efficient if some a priori knowledge is available about parameter and model uncertainties (Goel, 1988; Kimes, 2000; Verstraete et al., 1996). This knowledge specifies which target properties are the most significant determinants of spectral radiance observed in a specific spectral region. To this end, either extensive and detailed experimental data or a model of radiative transfer in the soil-vegetation-atmosphere system can be used. A sufficiently realistic model makes exploration of a broad range of target and observation conditions easier and effective through a systematic analysis of the sensitivity of modeled spectral radiance.

For given parameters, a sensitivity study quantifies how much each parameter contributes to the observed spectral radiance. This indicates wavelength dependency and identifies spectral ranges (bands) containing the most information about specific parameters. Identifying which target properties (parameters) control spectral radiance at a given wavelength and which ones have a negligible influence on spectral radiance at the same wavelength is very useful for quantitative remote sensing. For instance, identification of the most influential parameters on existing measurements of radiance helps to identify retrievable parameters (Bicheron and Leroy, 1999; Ceccato et al., 2002; Kimes, 2000; Mu et al., 2008). Furthermore, knowing the response of spectral radiance to biophysical parameters helps to determine appropriate spectral band combinations for the estimation of parameters of interest (Goel and Thompson, 1985; Kimes, 2000). An analysis of the sensitivity of modeled spectral radiance to target properties can address the issues mentioned above.

There is a variety of methods to conduct Sensitivity Analysis (SA) and different aspects of SA should be considered. Consensus about an exact terminology does not seem to exist yet (Cacuci et al., 2005). We have distilled from the literature a conceptual scheme about aspects and methods of sensitivity analysis. We may distinguish three aspects of SA briefly reviewed in the following paragraphs.

3.1.1. Sampling of the parameter space

SA may be carried out by exploring the neighbourhood of a single location in the parameter space (local SA) or by considering a number and distribution of samples sufficient to characterize reliably the entire parameter space (global SA). Evaluation of sensitivity at a single location or at a limited number of locations can be useful to evaluate well-defined target and observation conditions. In general, a systematic exploration of the parameter space is required. The ideal solution therefore would be to employ a full factorial design, i.e. testing all possible combinations of parameter values, to explore the entire parameter space. However, in the specific case of radiative transfer in the Soil-Vegetation-Atmosphere system, full factorial design is not practical. In some cases, an approximation of the full factorial design can be achieved with a reduced number of samples, using a fractional factorial design (Box et al., 1978). When only a fraction of all

possible combinations is considered, the distribution of samples is important to select an appropriate and representative sample set. In fact, sample size and sampling scheme (distribution of the samples) determine how much reliable information can be extracted from SA (Campolongo et al., 2007). Efficient sampling of the parameter space requires some a priori knowledge of the probability distribution of parameter values to adapt the sampling of the parameter space to the likely parameter values. This ensures that the unlikely parameter values and unlikely combinations are not given equal weight to the more likely ones.

3.1.2. Variation of parameters

We may change the values of parameters “*One (parameter) At a Time*” (OAT) or we may change “*All selected relevant Parameters Simultaneously*” (APS). The OAT approach has been the most frequently used approach in both remote sensing (Asner et al., 2000; Bach and Verhoef, 2003; Barton and North, 2001; Bicheron and Leroy, 1999; Peres and Da-Camara, 2004; Privette et al., 1994; Wang et al., 2008; Yao et al., 2008) and other fields (see (Saltelli et al., 2008)) because of its simplicity and inexpensive computational time. The OAT approach in remote sensing basically measures the sensitivity to a specific parameter by calculating discrete partial derivatives of spectral reflectance/radiance with respect to the input parameters (target and observation conditions). The APS sensitivity analysis scans the entire parameter space, for example with a Monte Carlo approach, to explore the possible range of variation for all parameters. In an APS exercise, all the parameters are varied simultaneously which provides information on the possible interactions among them as well. Although not extensive, the literature does contain a few studies that applied APS methods to quantify the sensitivity of output radiance/reflectance to input parameters of interest in remote sensing (Bacour et al., 2002; Ceccato et al., 2002; Morris et al., 2008; Pingheng and Quan, 2011)

3.1.3. Sensitivity measures

Measures of sensitivity for local sampling of the parameter space are limited to deterministic approaches such as partial derivatives. In the more general case of the exploration of the entire parameter space, statistics have to be defined and calculated to measure the sensitivity over a large number of sample points and for all parameters considered (Cacuci et al., 2005). With this approach, the output variance is decomposed into fractions of total variance which quantify the contribution of one or more parameters to the output variance. Many statistical sensitivity measures are currently in use; well-known are correlation-based methods (Saltelli and Marivoet, 1990), regression-based (Rabitz and Alis, 1999), variance-based sensitivity measures (e.g., Fourier Amplitude Sensitivity Test, FAST (Cukier et al., 1973), Sobol's method (Sobol, 1993; Saltelli, 2002) and more recently density-based methods (Borgonovo, 2006). These methods present elaborate and accurate sensitivity measures in which simultaneous parameter variation and robust statistical measures are combined. However, they are computationally expensive and complex because of the required large number of model evaluations (Saltelli et al., 2008).

The computational burden of a coupled surface-atmosphere radiative transfer (RT) model run depends strongly on the calculation mode and the accuracy of the compu-

tation. As an example, the coupled Soil-Leaf-Canopy RT model SLC (Verhoef and Bach, 2007) and MODTRAN (Berk et al., 1999, 1998) run may range from a few seconds, in a very simple case, to several minutes running the atmospheric code in an accurate mode. This makes the use of sophisticated methods impractical. The challenge addressed here is how to design a method to estimate sensitivities with an accuracy comparable to sophisticated global methods but with much less computational load. Morris (1991) proposed the elementary effect method as a screening method to identify a subset of non-influential inputs among a large number of parameters at a low computational cost. Though reducing the computational load, screening methods still suffer from some problems associated with the random sampling strategy which will be discussed in § 3.3.2.1. Moreover, the atmosphere influences Top-Of-Atmosphere (TOA) radiance considerably. In order to give an indication of the impact of the atmosphere on the sensitivity of different spectral bands to the input parameters, we also investigate the sensitivity of Bottom-Of-Atmosphere (BOA) reflectance to compare the results with the TOA radiance sensitivities.

This study aims at addressing four issues: (i) proposing an improvement of the design and sampling of screening methods for efficient sensitivity analysis of computationally expensive models (ii) using SA to identify influential and non-influential parameters on TOA radiance, (iii) comparison between TOA radiance sensitivity and BOA reflectance sensitivity to input parameters, and; (iv) investigating the effect of viewing and illumination geometry on TOA radiance sensitivity. In order to achieve these goals, we estimate sensitivity of TOA radiance and BOA reflectance to input parameters for a variety of sun-target-sensor observation geometries and three different atmospheric visibilities by both the proposed design and a variance-based method. We evaluate the efficiency and accuracy of the proposed design against the variance-based method.

The remainder of the paper is organized as follows. In Section 3.2, we introduce the approach used for the proposed design. Section 3.3.1 describes the radiative transfer models applied to simulate top and bottom of atmosphere radiance and reflectance. We discuss various aspects of sensitivity analysis and the methodologies used to estimate sensitivities in detail in Section 3.3.2. Section 3.4 presents the results of the evaluation of the proposed design and the results of the application of sensitivity analysis to identify influential and non-influential parameters. The comparison of TOA and BOA sensitivities and the effect of viewing and illumination geometry on TOA radiance sensitivity are also discussed in this section. Finally, Section 3.4.7 concludes the paper with a summary.

3.2. Approach

The analysis of the sensitivity of TOA radiance and BOA reflectance to target composition and architecture was carried out using the coupled SLC and MODTRAN radiative transfer models according to the approach described here.

3.2.1. Sampling of the parameter space

We applied the Sobol sequence generator (Sobol, 1993) to select a number (n) of base-line points in the parameter space. Sobol's sequence generator distributes new sample points using the location of previous points. This maximizes the uniformity of the sam-

pling and, unlike random sampling, prevents gaps or clusters to appear. These sample points are distributed within a $k - dimensional$ space, where k is the number of the input parameters.

3.2.2. Variation of parameters

The values of parameters at a baseline point are perturbed sequentially one at a time (see Figure 3.1a). Each step reaches a new point in the parameter space that is different from the previous sample point in only one dimension (one input parameter). The procedure continues until all input parameters are perturbed once and ends up at a new sample point which is different from the starting point. In this way for each baseline point, $k + 1$ new points are constructed sequentially to form a trajectory (i.e. a sequence of sample points) in the parameter space. Having n baseline points, at the end, there are n trajectories comprising $n(k + 1)$ sample points. The cost of the method (the number of required model runs) is then $n(k + 1)$.

3.2.3. Measures of sensitivity

Along a trajectory, the ratio of the variation in the output radiances of two successive sample points to the variation in the input parameter itself is calculated. This is the measure of the effect of the perturbed parameter along that segment of the trajectory. To compute sensitivities of spectral radiance to a certain input parameter over the entire sample space, the mean value and standard deviation of these ratios are calculated for each wavelength. Furthermore, a confidence level of 95 percent has been set for each sensitivity index to ascertain that the estimated results are consistent. This has been done by bootstrapping analysis. To evaluate the proposed design, we have compared it with the variance-based method. The comparisons are done on the basis of both direct comparison of spectral sensitivity and of parameter ranking. In the latter case, sensitivity results are transformed into ranks in order of importance and the correlation coefficients of the ranks, estimated by *Kendall's tau* approach (Abdi, 2007), are compared.

3.3. Methods and data

3.3.1. Top-Of-Atmosphere (TOA) radiance

TOA radiance is defined as a combination of surface reflectance, atmospheric effects and target's surroundings. This combination can be modeled effectively using the four-stream radiative transfer theory proposed by Verhoef and Bach (2003b, 2007, 2012).

$$L_{TOA} = \frac{E_s^0 \cos(\theta)}{\pi} \left[\rho_{so} + \frac{\tau_{ss}\overline{r_{sd}} + \tau_{sd}\overline{r_{dd}}}{1 - \overline{r_{dd}}\rho_{dd}} \tau_{do} + \tau_{ss}r_{so}\tau_{oo} + \frac{\tau_{sd} + \tau_{ss}\overline{r_{sd}}\rho_{dd}}{1 - \overline{r_{dd}}\rho_{dd}} r_{do}\tau_{oo} \right] \quad (3.1)$$

The definitions are given in Table 3.1; the overbars indicate spatial filtering over the surroundings of the target to account for the adjacency effect. The four successive summands on the right-hand side correspond to the contributions related to (i) target-independent atmospheric path radiance, (ii) adjacency effects, (iii) directly reflected solar illumination from the target, and (iv) directly reflected sky illumination on the target. The four-stream approach requires four surface reflectance factors plus seven atmospheric coefficients to simulate TOA radiance (Table 3.1). The surface reflectance

components are calculated by the SLC radiative transfer model and the atmospheric parameters are calculated by the MODTRAN atmospheric model. We have neglected the adjacency effect here since we are calculating TOA radiance for a single target. Surface bidirectional reflectance simulated by the SLC has also been used for the BOA reflectance sensitivity analysis.

3.3.1.1. Soil-Leaf-Canopy (SLC) RT model

The integrated Soil-Leaf-Canopy RT model SLC (Verhoef and Bach, 2007) was used to calculate top-of-canopy reflectance. SLC simulates TOC reflectance spectra over the spectral range between 400 and 2500 nm for arbitrary sun-target-sensor geometries. The model comprises structural and optical properties of the canopy, leaf and soil and the observation and illumination geometry. In fact, SLC is a four-stream extended version of the SAIL RT model (Verhoef, 1984) which uses four fluxes, including direct solar flux, diffuse downward flux, diffuse upward flux and directly observed flux (radiance). The model generates as outputs four reflectance factors of the canopy plus two canopy absorptances (Verhoef and Bach, 2007). The four canopy reflectances are r_{so} , r_{do} , r_{sd} and r_{dd} in Table 3.1 and the two canopy absorptances are canopy absorptance for direct solar incident flux and canopy absorptance for hemispherical diffuse irradiance.

Table 3.1: Variables modeled by SLC and MODTRAN used in the study

Variable	Description	RT model
L_{TOA}	TOA radiance	-
r_{so}	surface bidirectional reflectance factor	SLC
r_{do}	surface hemispherical-directional reflectance for diffuse incidence	SLC
r_{sd}	directional-hemispherical reflectance over surroundings	SLC
r_{dd}	bi-hemispherical reflectance over surroundings	SLC
ρ_{so}	TOA atmospheric bidirectional reflectance	MODTRAN
ρ_{dd}	BOA spherical albedo of the atmosphere	MODTRAN
τ_{ss}	direct atmospheric transmittance from the sun to the ground	MODTRAN
τ_{oo}	direct atmospheric transmittance from the ground to the sensor	MODTRAN
τ_{sd}	diffuse atmospheric transmittance from the sun to the ground	MODTRAN
τ_{do}	diffuse atmospheric transmittance from the ground to the sensor	MODTRAN
E_s^o	extraterrestrial solar irradiance on a plane perpendicular to the sunrays	-
θ_s	local solar zenith angle	-

Unlike its predecessors, SLC can treat the soil background as an anisotropic reflector. To simulate soil reflectance and its variability with moisture, a non-Lambertian extended version of Hapke's soil BRDF model (Hapke, 1981) containing the hotspot and soil moisture effects has been incorporated. The PROSPECT leaf reflectance model (Jacquemoud and Baret, 1990) is applied to compute transmittance and reflectance of green and brown leaves, in a version that can consider brown pigments (Verhoef and Bach, 2003b). The 4SAIL2 model (Verhoef and Bach, 2007) is employed to simulate canopy reflectance as a two-layer structure canopy reflectance model where a crown clumping effect (as in forests) is taken into account. The clumping effect is described by two additional parameters; vertical crown coverage (Cv) and tree shape-factor ($Zeta$). The latter is equal to the ratio of crown diameter to crown height. Furthermore, two parameters are used in

4SAIL2 to characterize the mixture of green and brown leaves in the canopy, namely the fraction of brown leaf area (fb) and a dissociation factor ($Diss$). When all green leaves are in the top layer and all brown leaves are laid down in the bottom layer, the dissociation factor is equal to 1. In case of dissociation equal to zero, all leaves are homogeneously mixed over the two layers.

Table 3.2: Input parameters of the SLC model

Parameter	Interpretation	Unit	min	max
$Hapke_b$	Hapke phase function parameter b	[-]	0.5	1
$Hapke_c$	Hapke phase function parameter c	[-]	0.3	1
$Hapke_h$	Hapke hot spot width parameter	[-]	0.05	0.80
$Hapke_{B0}$	Hapke hot spot magnitude parameter	[-]	0.05	0.80
SM	Soil moisture percentage	[-]	0.05	0.60
N_g	Mesophyll Structural parameter in Prospect, green leaves	[-]	1	2.5
Cab_g	Chlorophyll content in Prospect, green leaves	$\mu g/cm^2$	10	80
Cw_g	Water content in Prospect, green leaves	g/cm^2	0.001	0.1
Cdm_g	Dry matter content in Prospect, green leaves	g/cm^2	0.001	0.01
Cs_g	Senescence factor Prospect, green leaves	[-]	0.001	0.9
N_b	Mesophyll Structural parameter in Prospect, brown leaves	[-]	1	3
Cab_b	Chlorophyll content in Prospect, brown leaves	$\mu g/cm^2$	20	90
Cw_b	Water content in Prospect, brown leaves	g/cm^2	0.001	0.1
Cdm_b	Dry matter content in Prospect, brown leaves	g/cm^2	0.001	0.01
Cs_b	Senescence factor Prospect, brown leaves	[-]	0.001	0.9
LIDFa	LIDF parameter a, which controls the average leaf slop	[-]	-1	1
LIDFb	LIDF parameter b, which controls the distribution's bimodality	[-]	-1	1
Diss	Layer dissociation factor	[-]	0.1	0.9
Zeta	Tree shape factor	[-]	0.1	0.9
Hot	Hot spot size parameter	[-]	0.001	0.1
fb	Fraction brown leaf area	[-]	0	1
Cv	Vertical crown cover percentage	[-]	0	1
LAI	Total (green+brown) leaf area index	m^2/m^2	0	6
SZA	Sun Zenith angle	degree	-	-
VZA	Viewing zenith angle	degree	-	-
RAA	Relative azimuth angle	degree	-	-

The 4SAIL2 model accuracy has been verified by comparison against other models in the RAMI project (Widlowski et al., 2007) and with satellite and ground measurements (Verhoef and Bach, 2007). In the RAMI-3, the 4SAIL2 is shown to be in good agreement with the ensemble of all other models with less than 4% difference in BRDF simulations. Verhoef and Bach (2007) have demonstrated that the SLC model fit CHRIS-Proba data of the Upper Rhine Valley in Germany for different types of vegetations and bare soil with an average RMS error of 1.6% for nadir viewing, 2.3% for $\pm 36^\circ$ and 3.3% for oblique observations with $\pm 55^\circ$ between measured and simulated reflectances. SLC requires 26 input parameters (Table 3.2) where in this study the simulations are done for a range of sun-target-sensor geometries. For more details, the reader is referred to Verhoef and Bach (2007).

3.3.1.2. MODTRAN (MODerate resolution TRANsmittance and radiance code)

MODTRAN is a state-of-the-art code developed initially from the LOW resolution TRANsmittance 7 (LOWTRAN 7) model. It models scattering and absorption effects in the atmosphere with high accuracy and high spectral resolution up to 1 cm^{-1} . The scaled DIS-ORT (DIScrete Ordinate Radiative Transfer) algorithm is integrated for accurate computations of atmospheric multiple scattering and the correlated k algorithm is applied for regions with significant absorption effects (Berk et al., 1998). All these features make MODTRAN a reliable candidate for realistic simulation and analysis of remote sensing measurements. MODTRAN is well-suited for both at-sensor radiance simulation (Guanter et al., 2009; Laurent et al., 2011a; Schlapfer and Nieke, 2005; Verhoef and Bach, 2007, 2012) and for atmospheric correction (Adler et al., 1999; Schlapfer and Richter, 2002) from the UV to thermal infrared wavelengths. In the current study, the MODTRAN code was used to construct a look-up table of six atmospheric coefficients in Eq 3.1 for a number of different atmospheric scenarios.

3.3.2. Sensitivity analysis

This section presents the theoretical basis and the knowledge necessary for the reader to understand different aspects of sensitivity analysis. Following our procedure outlined in the introduction, we discuss different aspects of the two methods for sensitivity analysis; *the variance-based method* and *the proposed improvement*. Each subsection is devoted to a specific aspect of sensitivity analysis and relevant methodologies are described in detail.

3.3.2.1. Sampling of the parameter space

Random sampling, used in the *Morris* screening method, is simple and perhaps the most well-known amongst sampling strategies. Although widely used, assuming uncorrelated sample points might lead to clusters and gaps in the distribution of samples and to poorly distributed samples across the parameter space. This is more likely when the number of sample points is small relative to the number of input variables. Stratified sampling partly copes with this problem but still distributes samples randomly over sub-spaces. In fact, there exists a relatively high discrepancy between sample sets generated by random sequences in high dimensional spaces (Saltelli et al., 2008). The discrepancy of a sequence is low if the number of points in the sequence falling in an arbitrary set B is almost proportional to the measure of the set B . Low-discrepancy sequences offer a more effective way to sample the parameter space uniformly while working with high dimensional spaces. *Sobol* sampling is a low-discrepancy sequence that generates a uniform distribution in probability space. This method generates a new sample point with *a priori* knowledge of where the previous ones are located. In the first place, it samples from a multivariate uniform distribution, then goes back and fills in gaps left unsampled in repeated loops (Press et al., 2007). The sequence substantially improves the sampling in a multivariate parameter space. Among different sampling strategies, Sobol sampling has been recognized as one of the most appropriate sampling schemes to distribute samples over the parameter space while working with hypercube spaces (Saltelli et al., 2008). To apply Sobol sampling, the actual parameter values are scaled to a uniform distribution in $(0,1)$. This is characterized by the cumulative distribution function (CDF). If function F is

a cumulative distribution function with inverse function G , then $U = F(X)$ and $X = G(U)$ relates a random variable X with CDF F to a random variable U distributed uniformly on $(0,1)$.

3.3.2.2. Variation of parameters

To explore the parameter space, two parameter variation techniques have been employed. *Radial design sampling* and *winding stairs sampling* are applied with the variance-based method and the proposed design respectively. These strategies are explained in detail below.

Radial design sampling

Assume $A_1 = \{a_{11}, a_{12}, a_{13}, \dots, a_{1k}\}$ and $B_1 = \{b_{11}, b_{12}, b_{13}, \dots, b_{1k}\}$ are two synthetic canopy sample points generated by the Sobol sequence generator, where the first subscript denotes sample point number and the second subscript denotes input parameter number in a k -dimensional space. In radial design sampling, a new sample is drawn by moving a step in one direction within the parameter space each time. For instance, the first new sample point is generated by moving a step from the original point (A_1) towards the second point (B_1) in the direction of the first parameter, in which all the entries are from A_1 but the first one which is from B_1 and the new sample point is $A_B^1 = \{b_{11}, a_{12}, a_{13}, \dots, a_{1k}\}$. Similarly, the second new sample point is obtained by replacing the second parameter value of A_1 by the corresponding parameter value of B_1 so that $A_B^2 = \{a_{11}, b_{12}, a_{13}, \dots, a_{1k}\}$ and so on. This process continues until all parameters are varied once and forms a block. In other words, the radial design begins with an original point and moves away from the point in one direction each step, then returning back to the original point and moves in a different direction until all possible directions (the number of inputs) are accounted for. Hence, the k th sample point is $A_B^k = \{a_{11}, a_{12}, a_{13}, \dots, b_{1k}\}$. In such a design all the samples are symmetric to the first sample, which is characterized by a radial pattern (Figure 3.1b). Using radial design, for each sample point a block is constructed by a sample point from matrix A and k samples of A_B (Figure 3.2). Sensitivity indices are computed from n such blocks, each of size $(k + 1)$. Consequently, the total cost of the method is $n(k + 1)$.

Winding stairs sampling

The winding stairs sampling technique (Jansen, 1999; Saltelli et al., 2010) draws new sample points by moving a step in a new direction from the previous sample point (unlike the radial design that all the samples are a step away from the original point). Given the two samples A_1 and B_1 , the first new point is generated by moving a step away from A_1 in the direction of the first input parameter so that $B_A^1 = \{b_{11}, a_{12}, a_{13}, \dots, a_{1k}\}$. Likewise, the second point is drawn by moving a step from the previous generated sample B_A^1 in the direction of the second input parameter giving $B_A^2 = \{b_{11}, b_{12}, a_{13}, \dots, a_{1k}\}$, and so on. Therefore, the k th sample points is $B_A^k = \{b_{11}, b_{12}, b_{13}, \dots, b_{1k}\}$ that is the same as sample point B_1 . Winding stairs sampling begins with a sample point and moves away from that point each step in a new direction until all input parameters are perturbed once and ends up at a new point. New samples are drawn in a fixed cyclic order that constructs k new points after each cycle. Since the sample points differ in a single input

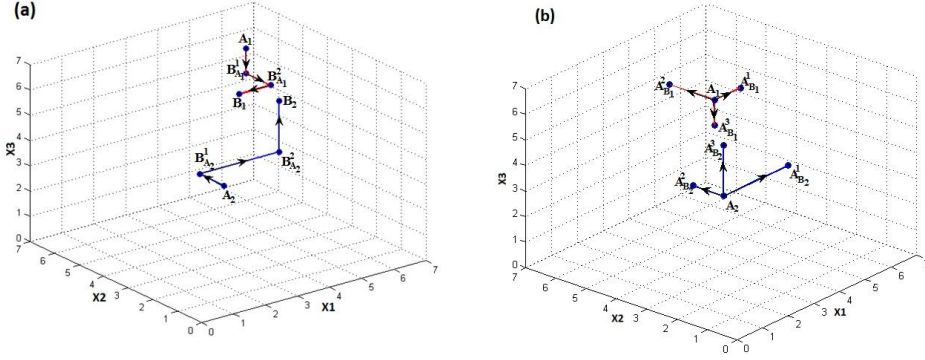


Figure 3.1: Examples of blocks in winding stairs sampling (a) and radial design sampling (b) in a three dimensional hypercube

parameter value, the design would ultimately have a stair-like form (Figure 3.1a). With winding stairs, for each sample point a block is built from matrix A and k samples of B_A (Figure 3.2). Sensitivity indices will be computed by n such blocks. Hence, the total cost of the method is $n(k+1)$. The winding stairs method makes a more balanced use of elements from matrices A and B , while a radial sampling block is mostly populated by elements from matrix A . In both designs, sampling blocks contain the same number of total-order sensitivity effects per each parameter which maintains the balance for each block internally (Saltelli et al., 2010). This helps to increase the number of blocks arbitrarily without worrying about the balance of the design. Overall, the winding stairs method has been shown to provide better estimates of sensitivity indices for small sample sizes (Chan et al., 2000).

$$\begin{aligned}
 A &= \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1k} \\ a_{21} & a_{22} & \cdots & a_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nk} \end{pmatrix} \\
 B &= \begin{pmatrix} b_{11} & b_{12} & \cdots & b_{1k} \\ b_{21} & b_{22} & \cdots & b_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ b_{n1} & b_{n2} & \cdots & b_{nk} \end{pmatrix} \\
 B_A &= \begin{pmatrix} b_{11} & a_{12} & a_{13} & a_{14} & \cdots & a_{1k} \\ b_{11} & b_{12} & a_{13} & a_{14} & \cdots & a_{1k} \\ b_{11} & b_{12} & b_{13} & a_{14} & \cdots & a_{1k} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ b_{11} & b_{12} & b_{13} & b_{14} & \cdots & b_{1k} \\ \hline b_{21} & a_{22} & a_{23} & a_{24} & \cdots & a_{2k} \\ b_{21} & b_{22} & a_{23} & a_{24} & \cdots & a_{2k} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ b_{21} & b_{22} & b_{23} & a_{24} & \cdots & a_{2k} \\ \hline \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ b_{n1} & a_{n2} & a_{n3} & a_{n4} & \cdots & a_{nk} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ b_{n1} & b_{n2} & b_{n3} & b_{n4} & \cdots & b_{nk} \end{pmatrix} \\
 A_B &= \begin{pmatrix} b_{11} & a_{12} & a_{13} & a_{14} & \cdots & a_{1k} \\ a_{11} & b_{12} & a_{13} & a_{14} & \cdots & a_{1k} \\ a_{11} & a_{12} & b_{13} & a_{14} & \cdots & a_{1k} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{11} & a_{12} & a_{13} & a_{14} & \cdots & b_{1k} \\ \hline b_{21} & a_{22} & a_{23} & a_{24} & \cdots & a_{2k} \\ a_{21} & b_{22} & a_{23} & a_{24} & \cdots & a_{2k} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{21} & a_{22} & a_{23} & a_{24} & \cdots & b_{2k} \\ \hline \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ b_{n1} & a_{n2} & a_{n3} & a_{n4} & \cdots & a_{nk} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & a_{n4} & \cdots & b_{nk} \end{pmatrix}
 \end{aligned}$$

Figure 3.2: An illustration of matrices A, B, A_B and B_A for winding stairs sampling (B_A) and radial design sampling (A_B)

3.3.2.3. Measures of sensitivity

An effective and robust sensitivity analysis method requires consideration of a set of sensitivity indices. These indices are a measure of the first-order effect (also known as

the main effect), second-order effects (the mutual interaction effect among parameters), higher order and the total-effect measures (the first-order effect plus all higher-order effects). With k input parameters, the entire number of first and higher-order effects would be $2^k - 1$ indices. Nevertheless, it is often desirable to compute only two sensitivity indices; first-order and total effect for each input parameter in a typical sensitivity analysis (Saltelli et al., 2010). These indices are addressed in the next section.

Sensitivity indices

Variance-based analysis is based on the decomposition of the total variance of the model output into components related to the different parameters and their interactions. The analysis relies on (i) the Sobol decomposition of a function, and (ii) the law of total variance (or variance decomposition formula) (Chen et al., 2004). Given an RT model $L_{TOA} = f(X)$, where L_{TOA} is the simulated radiance (we shall, for brevity, write L) and $X = \{x_1, x_2, x_3, \dots, x_k\}$ is a vector of k input parameters, X is assumed to contain independent components and have a joint density which is uniform over Ω^k , the k -dimensional unit hypercube, $\Omega^k = (X \mid 0 \leq x_i \leq 1; i = 1, \dots, k)$. The Sobol decomposition of the function $f(X)$ is given by (Sobol, 1993)

$$f(X) = f_0 + \sum_{i=1}^k f_i(x_i) + \sum_{1 \leq i < j \leq k} f_{ij}(x_i, x_j) + \sum_{1 \leq i < j < m \leq k} f_{ijm}(x_i, x_j, x_m) + \dots + f_{12\dots k} \quad (3.2)$$

where $i, j, m \in \{1, \dots, k\}$ and $f_0 = E(L)$ is the expected value of $f(X)$ over all parameters:

$$f_0 = E(L) = \int_{\Omega^k} f(X) dx \quad (3.3)$$

This expansion is a type of ANOVA decomposition. $f_i(x_i)$ is the first-order function for parameter x_i and $f_{ij}(x_i, x_j)$ indexes the second-order interaction of the parameters x_i and x_j . An input parameter has interactions with other parameters if its impact on the output depends on the value of the other parameters. All the terms in Eq 3.2 are orthogonal with zero mean. Therefore, by averaging out all the parameters but x_i minus the constant f_0 , one can obtain a decomposition only with respect to parameter x_i as follows;

$$f_i(x_i) = E(L|x_i) - E(L) = \int_{\Omega^{k-1}} f(x) d(x_{\sim i}|x_i) - f_0 \quad (3.4)$$

where $x_{\sim i}$ means all the input parameters except x_i . Similarly, a decomposition with respect to parameters x_i and x_j is

$$f_{ij}(x_i, x_j) = \int_{\Omega^{k-2}} f(x) d((x_{\sim ij} | x_{ij}) - f_i(x_i) - f_j(x_j) - f_0) \quad (3.5)$$

Therefore, the total variance $Var(L)$ can be written as the sum of the partial variances by squaring and integrating Eq 3.2 and, according to the orthogonality property of the decomposition terms in Eq 3.2 (Chen et al., 2004),

$$Var(L) = \sum_{i=1}^k V_i + \sum_{1 \leq i < j \leq k} V_{ij} + \sum_{1 \leq i < j < m \leq k} V_{ijm}(x_i, x_j, x_m) + \dots + V_{12\dots k} \quad (3.6)$$

where $V_i = Var_{x_i}(E_{x_{-i}}(L | x_i))$ is the contribution of x_i to $Var(L)$, $V_{ij} = Var_{x_{ij}}(E_{x_{-ij}}(L | x_{ij}))$ is the contribution of the interaction of x_i and x_j to $Var(L)$, and so on up to $V_{12\dots k}$, which is the contribution of the interaction of all the parameters to $Var(L)$. Eq 3.6 decomposes the total variance into distinct components related to each parameter and interaction. The measure of importance of a parameter can then be expressed as the expected reduction in the total variance, given that parameter, i.e., $E(Var(L) - Var((L | x_i)))$, which according to the law of variance is equal to V_i in Eq 3.6. Likewise, V_{ij} is the expected reduction in the total variance, given two parameters, x_i and x_j . Variance-based sensitivity indices are estimated as ratios between the partial variances and the total variance.

$$S_i = V_i / Var(L) \quad (3.7)$$

$$S_{ij} = V_{ij} / Var(L) \quad (3.8)$$

S_i is the main effect of parameter x_i on the total variance and S_{ij} is the second-order effect of x_i . The main effect indicates the relative importance of the parameter on the model output. This effect is additive on the model output and independent of the value of the other input parameters (Monod et al., 2006). A measure of the total-order effect (S_{Ti}) can be interpreted as the effect of each parameter on the output variance while all interactions with other parameters are taken into account. This denotes the main effect of a parameter and all other higher-order effects.

$$S_{Ti} = E_{x_{-i}}(Var_{x_{-i}}(L | x_{-i})) / Var(L) = 1 - (V_{-i} / Var(L)) \quad (3.9)$$

Assuming three parameters, the total effect index of a parameter as reported by Saltelli et al. (2010) is represented by a sequence of sensitivities;

$$S_{T1} = S_1 + S_{12} + S_{13} + S_{123} \quad (3.10)$$

An ideal sensitivity method must be able to take into account the interaction among different input parameters; in particular for nonlinear models. This demands quantification of all effects and calculation of all indices defined above with a sufficient number of samples. The computation of the sensitivity indices of the applied methods is discussed in the following sections.

Sensitivity indices of the variance-based method

Among global statistics analysis methods, variance-based methods are often referred to as accurate global methods in the literature (Saltelli et al., 2010). For this study, the variance-based approach, as described in Saltelli et al. (2010), was evaluated as a reference to measure first and total sensitivity indices. The method implements the radial design sampling technique described in § 3.3.2.2. The blocks generated by the radial design method are used to construct conditional variances and the total variance of the

model. Further, sensitivity indices are derived from such variances. The first-order sensitivity index is given by

$$S_i = \frac{\frac{1}{n} \sum_{j=1}^n f(B)_j (f(A_B^i)_j - f(A)_j)}{Var(L)} \quad (3.11)$$

Here, A and B are the two independent sampling matrices, A_B^i is the design matrix constructed by the radial design sampling in § 3.3.2.2 (Figure 3.2), where all columns are from A but the i th column is from B and $f(\cdot)$ denotes the evaluation of the RT model at sample points (output radiance). Likewise, the total indices were estimated with Jansen's formula (Jansen, 1999), which has been shown to usually perform best among available formulas (Saltelli et al., 2010).

$$S_{Ti} = \frac{\frac{1}{2n} \sum_{j=1}^n \left(f(A)_j - f(A_B^i)_j \right)^2}{Var(L)} \quad (3.12)$$

Sensitivity indices in the proposed method

The proposed method combines the Sobol sampling scheme with winding stairs parameter variation (see § 3.3.2.2). The Sobol scheme efficiently distributes the sample points over the entire parameter space and avoids gaps and clusters. This gives a fairly good exploration of the parameter space even with a limited number of sample points. The ratio between the variation in the output radiance of two successive sample points and the variation in the input parameter itself is calculated. Therefore, along a trajectory, k ratios are calculated, one for each parameter. Having n such ratios for each parameter, one can calculate statistics to assess sensitivity. We have used the mean of the absolute value of all these ratios for each parameter as the total-order effect of that parameter.

$$S_{Ti} = \frac{\sum_{t=1}^n \left| \frac{f_{(i+1,t)}(x_1, \dots, x_k) - f_{(i,t)}(x_1, \dots, x_k)}{dx_i} \right|}{n} \quad (3.13)$$

where t is trajectory number, n stands for the number of trajectories, dx_i is the variation in parameter i and $f(i, t)$ denotes the radiance of sample point i . Furthermore, the standard deviation of the ratios for each parameter has been calculated to represent the degree of nonlinearity of the given parameter.

3.3.3. Bootstrap condence intervals

A sensitivity study is incomplete without an understanding of the accuracy of the estimated indices. High uncertainty might emerge in the estimation of sensitivity indices due to the nature of sampling strategy used in sensitivity analysis (Archer et al., 1997). The bootstrapping approach (Efron and Tibshirani, 1993) was applied with blocks (i.e. blocks of sample points) to estimate confidence bounds on the sensitivity indices. In this approach, the generated samples are resampled with replacement many times to create a number of bootstrap replicate data sets and form a distribution of sensitivity indices. The percentile method (Efron and Tibshirani, 1993) is then utilized to construct

bootstrap confidence intervals in which for a 95% confidence interval, the lower and upper 2.5% percentiles of the generated distribution of the bootstrap are used. It is also worth noting that the bootstrap resampling comes at no further cost, because model evaluation of all blocks is already done.

3.3.4. Evaluating parameter ranking

Since the ultimate goal is to identify influential and non-influential parameters, i.e. ranking the input parameters based on their importance, a rank transformation is done by simply replacing the sensitivity scores of all methods with their respective ranks and then assessing the Kendall correlation between different methods on the ranks rather than the corresponding sensitivity values. Hence, if the number of parameters is k , then the largest score among the sensitivity values is assigned rank 1, the next largest value is assigned rank 2, etc. The Kendall correlation coefficient (also known as Kendall's tau (τ) coefficient) is a non-parametric test to measure the strength of the relationship between two ranked samples (Abdi, 2007). τ varies between -1 and 1 and yields a positive correlation if the measured ranks of both methods increase together, whilst mismatching between two ranks results in a negative correlation. Having two sets of ranks each containing k parameters, there are $k(k-1)/2$ possible comparisons of pairs (X_i, Y_i) and (X_j, Y_j) . Kendall's tau is given by

$$\tau = \frac{N_C - N_D}{\frac{1}{2}k(k-1)} \quad (3.14)$$

where N_C is the number of concordant pairs and N_D stands for the number of discordant pairs. This test provides a consistent measure of the similarity between ranked parameters. This measure reflects well the importance of agreement on the top ranks.

3.3.5. Setting up the sensitivity experiments

All input parameters and their ranges of variation were selected identically for all the sensitivity experiments. A set of biophysical parameter values was derived from the literature and field measurements with the goal of covering a wide range of vegetation conditions. This set was used to define the range of variability of each parameter (Table 3.2). The sensitivity analysis was conducted with a variety of different sun-target-sensor geometries. During each experiment, two Solar Zenith Angles (SZA) were set at 30° and 60° corresponding to high and low sun elevations, and View Zenith Angle (VZA) was allowed to take on five values of 0°, 15°, 30°, 45° and 60° and Relative Azimuth Angle (RAA) two values of 30° and 150°. Thus, there were 20 sets of sun-target-sensor geometries. Furthermore, this test was repeated for three different atmospheric profiles with visibility values at 10, 23 and 50 km, representing a very hazy, moderate and clear sky respectively, to quantify the effect of solar/view geometry and the atmosphere on the sensitivity results. The acquisitions were simulated with the observation configuration listed in Table 3.2. The spectral sampling of the simulations was adjusted to 1 nm, i.e. 2101 contiguous spectral bands were taken between 400 and 2500 nm. These spectral bands were then convolved to match the Hyperion sensor characteristics. In order to mimic actual Hyperion images, several spectral bands were removed due to water absorption, intersection bands and very low signal so that eventually 196 spectral bands were used in

the 400-2400 nm region for further analysis. Therefore, the spectral bands corresponding to regions between 1350 and 1420 nm, 1800 and 1930 nm, and above 2400 nm were removed and are not included in the graphs.

3.4. Results and discussion

3.4.1. Evaluation of the proposed design

The performance of the proposed design was compared to the variance-based method based upon the ranking of the most influential and non-influential input parameters in order of importance at a given wavelength. A high correlation value (see Eq 3.14) between two methods indicates high degree of similarity in the ranking of the parameters. While applying Sobol's sequence, additional uniformity can be reached by increasing the sample size by taking $n - data$ points where $n = 2^a$ and a is an integer (Sobol, 1967). Based on this recommendation, n was set to 2^{11} resulting in $2048(23 + 1) = 49,152$ synthetic canopies to calculate the first-order and total-order sensitivity indices in the variance-based approach. Preliminary analysis on the number of sample points showed that the assessed sensitivity indices with this sample size are highly correlated to the ones with larger sample sizes. Therefore, the sample size is deemed adequate to give reliable sensitivity indices. As stated in § 3.3.3, since bootstrapping analysis comes at no extra cost, the results were resampled 10000 times (with replacement) to have reliable estimates. In order to select a proper number of samples for the proposed design, we investigated its convergence behavior in terms of sample size. Six different number of trajectories at 10, 20, 50, 70, 100 and 200, corresponding to 240, 480, 1200, 1680, 2400 and 4800 sample points respectively, were taken to inspect whether an increasing numbers of trajectories would effectively improve the performance of the method. The results revealed that increasing the number of trajectories improves the correlation between the proposed design and the variance-based method to some extent. However, the proposed design tends to converge toward an almost stable average correlation of 92 percent with the variance-based method and no significant difference is found by increasing the number of trajectories beyond 50. This suggests that a good level of agreement may be reached with this number of trajectories. Therefore, the number of 50 trajectories was selected for further analysis in the study, hence the total cost of the method is $50(23 + 1) = 1200$ simulations.

Figure 3.3 illustrates two pairwise comparisons between the proposed design and the variance-based method in terms of parameter ranking. Two solar/view geometries are plotted, a nadir view with low solar zenith angle and very high view and solar zenith angles. It is shown that the method is in good agreement with the variance-based method for the entire spectrum. However, the results indicate that the correlation is slightly higher from the visible to the near-infrared (~ 1400 nm) region. An explanation for this is the fact that Kendall's τ is more sensitive to agreement in the top ranks than in the lower ranks. Therefore, over the visible to near-infrared region where there are a group of dominant parameters with distinguished sensitivity values that attain top ranks, both methods can equally rank the parameters and a higher correlation is to be expected, whereas for the rest of the spectrum there are more parameters with similar low sensitivity values which potentially leads to less similarity in parameter ranking. The corre-

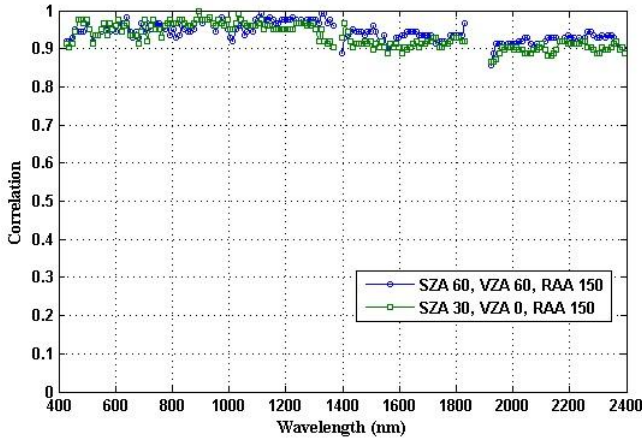


Figure 3.3: Kendall tau correlation coefficient between the proposed design (1200 model runs) and the variance-based method (49,152 model runs). The blue line represents solar zenith angle of 60°, viewing zenith of 60° and relative azimuth angle of 150°; the green line represents solar zenith angle of 30°, nadir viewing angle and relative azimuth angle of 150°

lation coefficients, averaged over the entire spectrum, are 0.92 and 0.93 for the low and high zenith angles, respectively. In general, for all the solar/view geometries and different atmospheric profiles applied in this study, the mean correlation coefficients were 0.91 to 0.93. The results demonstrate that the proposed design is reasonably accurate in parameter ranking while applying only 1200 model runs versus 49152 model runs with the variance-based method.

3.4.2. Influential and non-influential parameters

Reliable quantitative information can be retrieved on a parameter, if that parameter is strongly related to the output radiance (Kimes, 2000; Verstraete et al., 1996). This implies that a parameter is retrievable if the sensitivity of output radiance to that parameter is significant. In other words, a high sensitivity value means that the parameter is responsible for a significant portion of the output variance of the radiance which leads to a greater chance of retrieval of that parameter. In an ideal case, the necessary and sufficient condition for an input parameter to be non-influential is that the main effect and the interaction effects with other parameters are zero, which shows that the contribution of the parameter on the output variance is zero. This condition allows assigning an arbitrary value to that parameter within its domain. In practice, input parameters with little effect can be treated as non-influential if their effect is very small compared to the other parameters for a given wavelength. For instance, chlorophyll strongly influences the visible spectrum by absorption while showing negligible effect in the shortwave infrared region. To assess the actual influence of a given parameter, both the main effect and the interaction effects among parameters have to be taken into account. To show the importance of interaction effects amongst input parameters, we have plotted in Figure 3.4 the sum of the first-order effects and total-order effects for a given solar viewing

geometry. The blue line represents the sum of all the total-order effects, the red line indicates the sum of the first-order effects and the green area is the interaction effects among parameters. It should be noted that the sum of first-order effects over all input parameters cannot exceed one, and does not equal one unless all the interaction terms are zero. By contrast, the sum of total-order effects over all input parameters is never less than one, and equals one only if all interaction terms are zero, because this sum includes every first-order effect once and every interaction term multiple times.

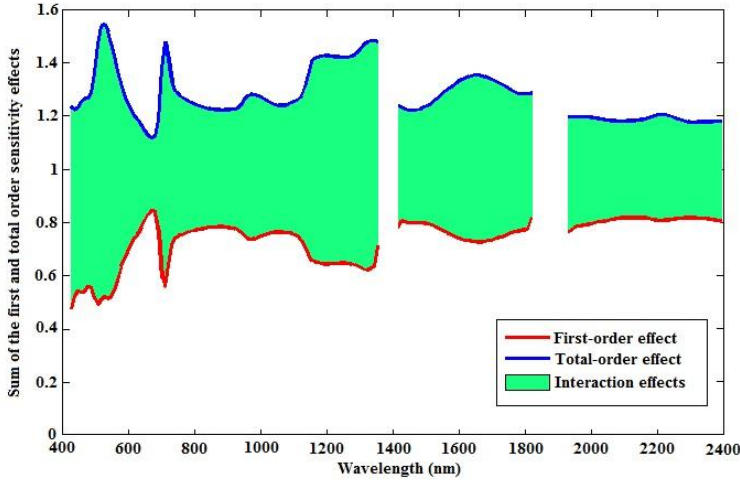


Figure 3.4: Sum of the first-order effects, interaction effects and total-order effects over all the parameters for nadir view angle and solar zenith angle of 30°

Figure 3.4 depicts that the sum of the first-order and total-order effects is almost symmetric with a few exceptions due to some round-off error. It is shown that the sum of the interaction effects among the input parameters reaches a maximum in the visible, and in particular near the green region ($\sim 550\text{nm}$) corresponding to a peak in the reflectance of vegetation. This means that a large portion of uncertainty in the output radiance is driven by interaction among the factors in this region. While the red-near infrared ($\sim 670\text{nm}$), corresponding to maximum vegetation absorption, seems to have the least impact on the interaction effects where approximately 85% of the output variance in TOA radiance is explained by the main effects. The possible conclusion is that the green channel is very sensitive to a number of parameters that are correlated and cause considerable interaction effects. But the red-near infrared ($\sim 670\text{nm}$) is only sensitive to a few dominant parameters (such as LAI, Cv and SM) and therefore it includes only the interaction effects of them.

Since the total-order effect of a parameter includes the first-order plus all the interaction effects, we have used total-order effect to identify the dominant and negligible input parameters. The total-order effects estimated by both methods are given in Figure 3.5 and Figure 3.6 for a solar zenith angle of 30° , nadir viewing zenith and relative azimuth angle of 150° . Figure 3.5 illustrates the most influential parameters and the in-

put parameters with the lowest sensitivity values are shown in Figure 3.6. Direct comparisons between sensitivity values estimated by both methods show that for some parameters the proposed design underestimates sensitivities. This happens if the sample space is small and the model is nonlinear. However, in general, there is good agreement between both methods for selecting influential and non-influential parameters at any given wavelength.

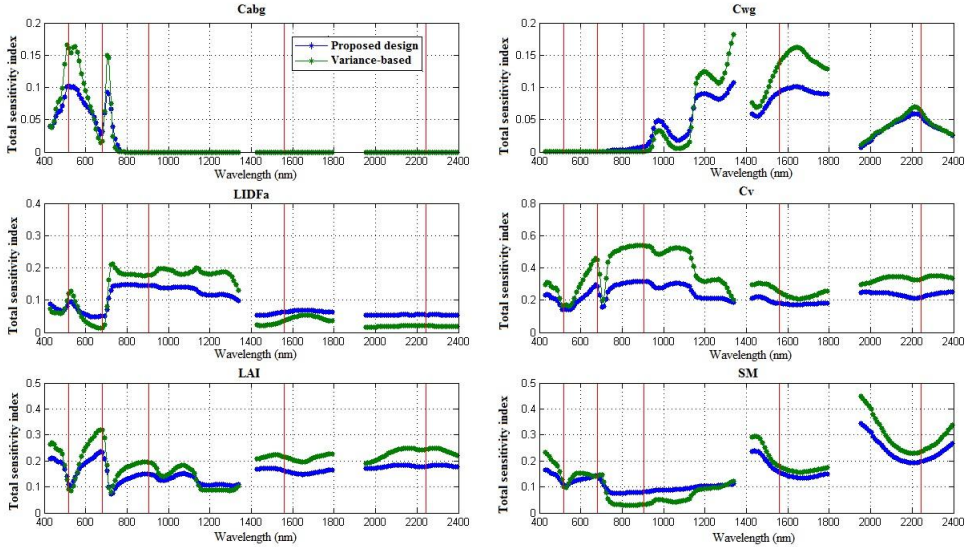


Figure 3.5: Total-order sensitivity effect of the most influential parameters for solar zenith angle of 30°, nadir viewing zenith angle and relative azimuth angle of 150°

3.4.3. Physically-based understanding of the radiative processes that govern the simulations

The radiation in the range from 400 to 700 nm is the photosynthetically active radiation for plants. Spectral features in this region are primarily controlled by leaf pigments and in particular chlorophyll concentration. Therefore, spectral radiance is most sensitive to chlorophyll content, senescence factor and other relevant parameters such as the fraction of brown leaf area (fb) and dissociation factor ($Diss$). The effect of chlorophyll content and senescence factor disappears beyond approximately 700 nm and 1000 nm respectively due to the fact that chlorophyll and other leaf pigments are transparent to infrared radiation. When the subscripts for green (g) and brown (b) leaves are not given, we mean both leaf types. Leaf mesophyll structure (N) parameter and dry matter content (Cdm), on the other hand, influence the near-infrared spectra depending on the relative thickness of the mesophyll. In general, the sensitivity of the observed radiance to N and Cdm is relatively small, especially for dry matter content which is less than 3% at its highest value. Cdm and N parameters also affect the short-wave infrared region.

Water content (equivalent water thickness (Cw)) has negligible impact on the visi-

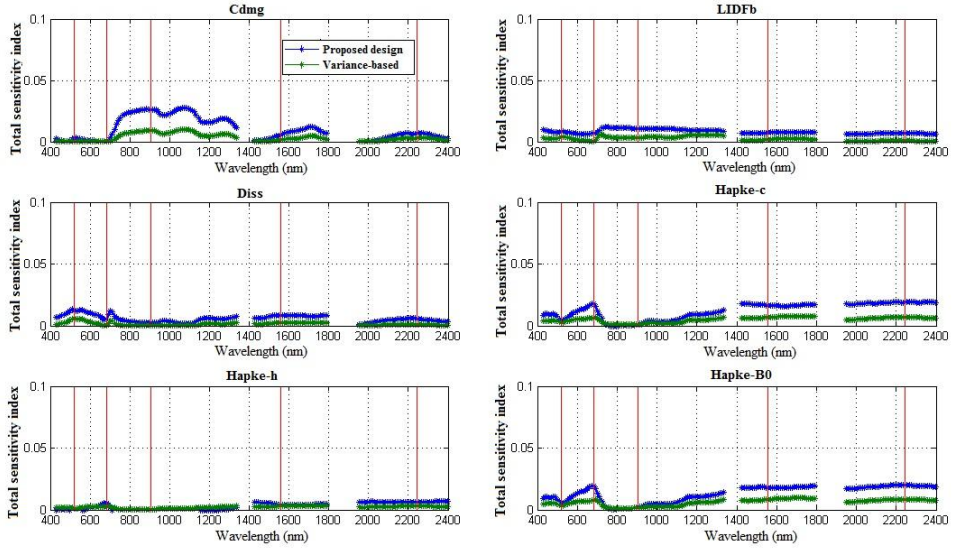


Figure 3.6: Total-order sensitivity effect of the input parameters with the lowest sensitivity values for solar zenith angle of 30° , nadir viewing zenith and relative azimuth angle of 150°

ble and the near-infrared but influences the shortwave infrared considerably because of radiation absorption by leaf water content. Water content is responsible for more than 10% of the output variance between 1200-1300 nm and 1500-1700 nm (Figure 3.5). Leaf area index (LAI) and vertical crown coverage (Cv) are very influential parameters affecting the output radiance over almost all the spectral bands. This is explained by the fact that LAI and Cv are the indicators of the presence and density of vegetation and determine radiation interception by the canopy. Even a small variation in the value of these two parameters causes some change in the observed radiance. Nonetheless, the highest sensitivity to LAI is seen in the red-near infrared where the maximum change in the absorption of radiation from vegetation occurs. The impact of LAI and Cv remain almost stable from 1400 nm onwards, while the most dramatic declines are seen around 550 nm and 700 nm because of the sharp peaks in the influence of chlorophyll and $LIDFa$ parameters. Similarly, an increase in the influence of water content causes a decrease in the impact of LAI and Cv .

Leaf inclination distribution function parameter a ($LIDFa$) controls the average leaf slope, which in turn controls radiation interception by the leaves and therefore is an important parameter contributing to the output radiance, but the parameter b that controls the distribution's bimodality is shown to be non-influential over almost the entire spectrum. The influence of $LIDFa$ goes up around 700 nm and remains steady until around 1300 nm when there begins a decline. This is due to the high infrared reflectivity of leaves which is controlled by $LIDFa$ parameter. Soil moisture affects the observed radiance at all wavelengths but its influence is larger for the shortwave infrared spectra. All the Hapke's soil parameters (except Hapke's phase function parameter b) and

hot-spot effect show very small effect on almost all the spectral bands (Figure 3.6). Soil parameters have a secondary effect (background effect) on the reflectance/radiance of a canopy which is generally low, especially with the increase of vegetation cover. There is another reason, however, that might explain the low effect of the three Hapke's parameters: $Hapke_{B0}$ and $Hapke_h$ parameters are only responsible for the soil's hot spot effect and with $Hapke_c$ parameter, they only have an influence on the bi-directional reflectance factor (r_{so} in Table 3.1). This implies that the effect of these parameters is marginal on the output radiance since in the four-stream approach, implemented in this study, four different reflectance factors are considered.

3.4.4. Detailed interpretations of the sensitivities of five Hyperion spectral bands

We have selected five Hyperion spectral bands (the vertical red lines in Figure 3.5 and Figure 3.6) as examples for more detailed interpretations of all the input parameters. The selected spectral bands are centered at 519, 681, 905, 1558 and 2244 nm in accordance to Hyperion spectral bands 17, 33, 55, 141 and 210 respectively. The results for the five spectral bands are summarized in Table 3.3 and Figure 3.7. Table 3.3 lists the sensitivity of each spectral band to all input parameters. Figure 3.7 also provides the total-order sensitivity index of these five bands with a comparison to the proposed design.

Parameters with zero value in Table 3.3 (and Figure 3.7) have simply no influence on the related spectral band. For instance, band 17 and band 33 are not sensitive to Cw and Cdm . This is because these two bands are located in the photosynthetic pigments region where variations in the amount of water content or cell structure do not impact the output radiance. On the other hand, band 141 is the best suited band to study Cw since it is located in a very sensitive region to variations in canopy water content. Aside from the ideal case, i.e. zero sensitivity value, one may decide to define a parameter as negligible according to the accuracy required. Measure of this accuracy can be defined with reference to a fixed number of decimal places, i.e. the number of digits following the decimal point. This can be interpreted as approximate with a precision equal to the number of zero-valued digits one can assume the parameter in question as negligible without affecting too much the output radiance. For instance in band 210, with a precision of two decimal digits, we may label N , Cab , Cdm , Cs , $Diss$, $LIDFb$, Hot and $Hapke_h$ as parameters with negligible effect. Likewise, Cw , Cdm , Hot and $Hapke_h$ are parameters for which band 17 is insensitive with three decimal digits precision. If a parameter is labeled as negligible for a spectral band, it means that the band cannot be used for the retrieval of that parameter.

This analysis is useful in the context of parameter retrieval problems to decide which parameters can be kept constant during retrieval. A further analysis of the sensitivity of each spectral band to input parameters can be of help in identifying which spectral band is more sensitive to a certain parameter. This, in turn, is translated into finding the optimal band selection in a parameter retrieval problem. As discussed before, based on the sensitivity concept, the spectral bands that present the highest sensitivity to a given parameter are more likely suitable for retrieval purposes than those with very small sensitivity values. This can be best demonstrated by employing an inversion algorithm, in which the results extracted from an optimal band selection are validated using ground

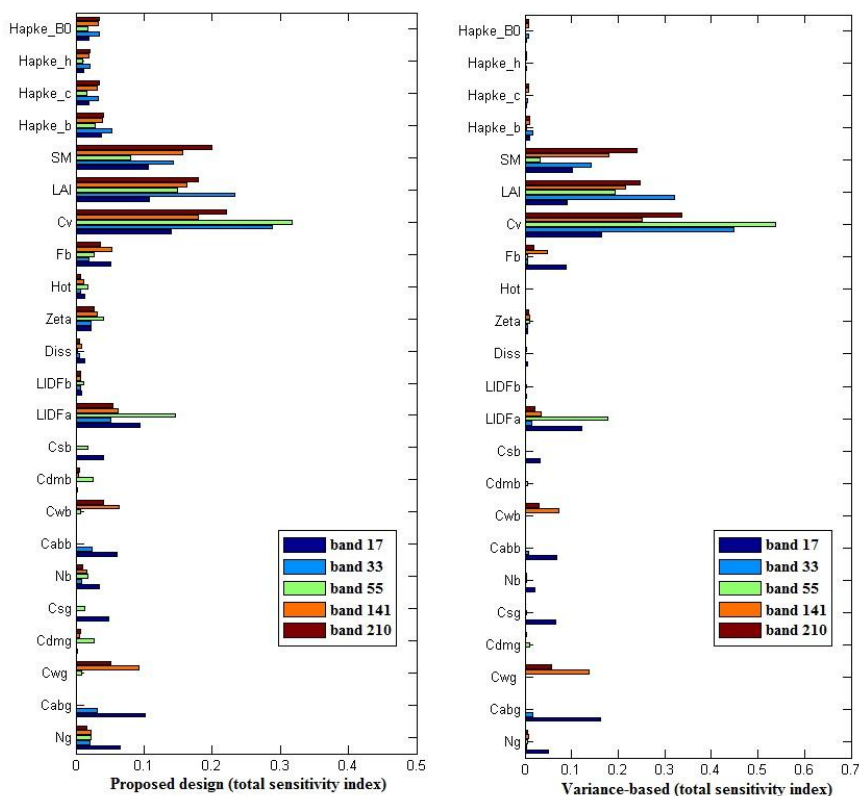


Figure 3.7: Total-order sensitivity effect of the five simulated Hyperion spectral bands

truth measurements. However, this is beyond the scope of this paper and will be addressed in future studies.

3.4.5. TOA radiance sensitivity vs BOA reflectance sensitivity

We have also performed the sensitivity analysis for BOA reflectance to investigate the impact of the atmosphere on the sensitivity values of input parameters. The atmosphere has a complicated influence on the observed radiance in the optical solar spectral range. This influence is specifically significant on visible and the infrared radiation. Two major effects of the atmosphere are scattering and absorption. Atmospheric absorption is primarily due to gaseous and aerosols absorption properties. The scattering effect is caused by molecules and aerosols (Kaufman and Tanre, 1996). We have used three different visibilities, as an indicator of aerosol load, at 10km , 23km and 50km characterizing hazy to clear atmospheres. A rural aerosol type and a mid-latitude summer atmosphere were selected and the water vapor content was assumed to be 2g/cm . Figure 3.8 compares the total-order sensitivity of BOA reflectance and two TOA radiance sensitivities for atmospheric visibilities of 10km and 23km . For the sake of clarity, we only plot the compar-

Table 3.3: Total-order sensitivity effect of the five simulated Hyperion spectral bands

Parameter	Band 17	Band 33	Band 55	Band 141	Band 210
N_g	0.0505	0.0039	0.0054	0.0088	0.0046
Cab_g	0.1611	0.0173	0.0000	0.0000	0.0000
Cw_g	0.0000	0.0000	0.0010	0.1371	0.0572
Cdm_g	0.0002	0.0000	0.0090	0.0016	0.0033
Cs_g	0.0656	0.0002	0.0026	0.0000	0.0000
N_b	0.0210	0.0017	0.0035	0.0040	0.0022
Cab_b	0.0687	0.0072	0.0000	0.0000	0.0000
Cw_b	0.0000	0.0000	0.0006	0.0724	0.0299
Cdm_b	0.0001	0.0000	0.0055	0.0008	0.0014
Cs_b	0.0316	0.0001	0.0017	0.0000	0.0000
LIDFa	0.1216	0.0137	0.1775	0.0354	0.0206
LIDFb	0.0037	0.0007	0.0034	0.0019	0.0009
Diss	0.0059	0.0005	0.0001	0.0026	0.0012
Zeta	0.0052	0.0045	0.0112	0.0100	0.0067
Hot	0.0016	0.0003	0.0021	0.0012	0.0005
fb	0.0885	0.0067	0.0061	0.0485	0.0194
Cv	0.1651	0.4494	0.5374	0.2520	0.3368
LAI	0.0898	0.3198	0.1935	0.2154	0.2466
SM	0.1014	0.1410	0.0324	0.1795	0.2403
$Hapke_b$	0.0112	0.0167	0.0035	0.0107	0.0099
$Hapke_c$	0.0027	0.0061	0.0013	0.0068	0.0069
$Hapke_h$	0.0012	0.0027	0.0006	0.0030	0.0031
$Hapke_{B0}$	0.0033	0.0075	0.0016	0.0084	0.0086

isions of some dominant parameters. Strong atmospheric absorption bands are omitted from the graphs and only BOA sensitivities are shown for these bands.

The measured sensitivities of BOA spectral reflectance are similar to the TOA radiance sensitivities with a few exceptions when the atmosphere is clear and visibility is high (Figure 3.8). When visibility decreases there are some significant differences between the measured sensitivities for BOA and TOA. It is not surprising that the most remarkable differences are seen in the visible spectra for dominant parameters driving the uncertainty in the output. It is well known that atmospheric scattering is more significant for visible wavelengths where the scattering modifies the propagation direction and causes gain on the radiation reaching the sensor. The hazier the atmosphere becomes, the larger the influence it has on the sensitivity to the input parameters. This difference is larger for parameters relevant to leaf pigments such as Cab and fb in the visible region. The results, as shown in Figure 3.8, indicate the influence of most parameters is less affected by the atmosphere for the shortwave infrared wavelengths. A possible explanation for this is that scattering continuously decreases from visible towards the infrared and consequently has less impact on the sensitivities. It is also evident from this figure that a unique pattern cannot be introduced so that visibility decreases or increases the

influence of a parameter similarly over the entire spectrum. This is due to the fact that a decrease in the sensitivity to a certain parameter causes an increase in the other sensitivities. These findings suggest that in general the sensitivity of TOA radiance to the input parameters in the case of clear atmosphere is similar to BOA reflectance sensitivity excluding the strong atmospheric absorption wavelengths.

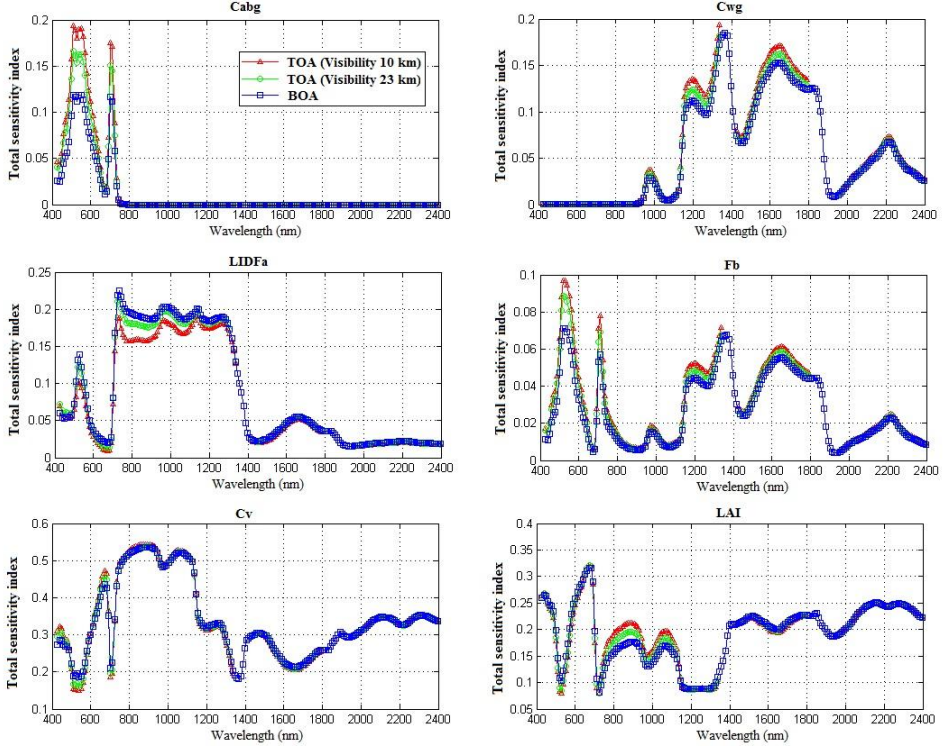


Figure 3.8: Total-order sensitivity of BOA reflectance and two TOA radiance sensitivities for atmospheric visibilities of 10 km and 23 km

3.4.6. Effect of viewing and illumination geometry on TOA radiance sensitivity

Canopy reflectance is anisotropic and exhibits variation in sensitivity values as a function of illumination and viewing geometries. The SLC is able to model anisotropic reflectance which makes it possible to investigate the impact of geometry on the sensitivity. The in-depth analysis of the geometry effect on the sensitivity and finding the optimal geometry configurations for parameter retrieval is out of the scope of the current study and will be described in a future studies. Here, we have plotted the spectral sensitivity for four different viewing/illumination directions in Figure 3.9 to give an impression about the influence of the sun-target-sensor geometry on the sensitivity of TOA radiance to two dominant parameters; Cv and LAI. The impact of anisotropy is wave-

length dependent. As shown in Figure 3.9, in general, for both parameters the observed difference between solar/view directions is not significant in the visible, while it is larger in the NIR and SWIR wavelengths. From 800 nm onwards, the difference in sensitivity for nadir view with SZA of 30° and SZA of 60° with a large VZA of 60° reaches more than 10% and 5% for Cv and LAI respectively. The sensitivity in the spectral range from 1400 nm to 1800 nm is very high at SZA of 30° with nadir view while from 700 nm to 1400 nm the lowest sensitivity is observed for this geometry. A possible explanation for this might be that increasing or decreasing the sensitivity value to one parameter affects the other sensitivities, for example, in the spectral region from 2000 nm onwards an increase in the sensitivity at the low solar/view angles to Cv causes a decrease in the sensitivity for the same geometry to LAI.

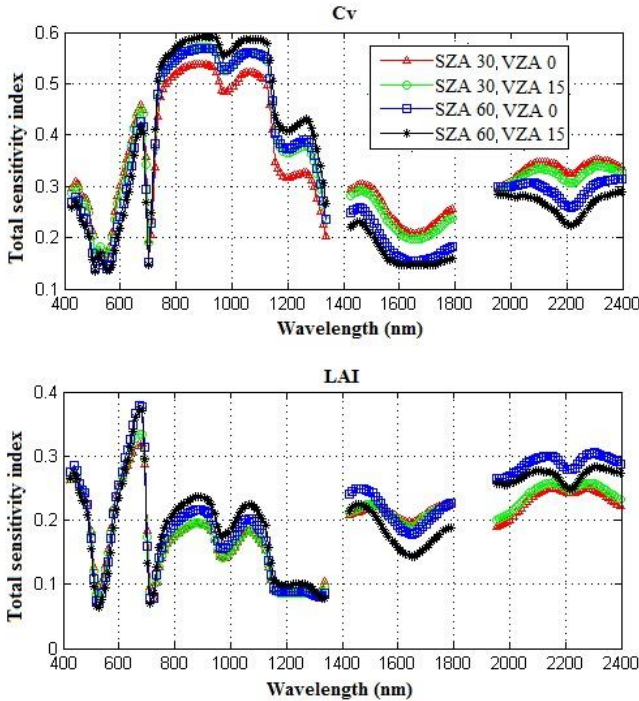


Figure 3.9: Comparison of the total-order sensitivity of TOA radiance to Cv (top) and LAI (bottom) for four viewing/illumination directions

3.4.7. Summary and conclusions

We assessed the sensitivity of TOA radiance and BOA reflectance of a soil-vegetation system to the input biophysical and biochemical parameters using the coupled Soil-Leaf-Canopy radiative transfer model SLC and MODTRAN. An improvement in the design and sampling of screening methods was proposed based on a Sobol sampling strategy and winding stairs parameter variation. The results demonstrated that the proposed

improvement is efficient in identifying dominant and non-dominant input parameters compared to the variance-based method with modest computational demands (only 1200 model runs against 49152 model runs in the variance-based method). In general, therefore, it seems that the proposed design can be used instead of complex global methods when the objective is to identify influential and non-influential parameters among many other parameters or with computationally expensive methods. In particular it can be used where it is necessary to have fast and appropriate sensitivity estimates of a coupled surface-atmosphere radiative transfer model at low computational cost.

Among 23 input parameters, crown coverage (Cv), leaf area index (LAI), leaf inclination distribution function ($LIDFa$) and soil moisture (SM) were found to be the most influential parameters driving the output variance of the radiance from 400 nm to 2500 nm with a few exceptions. Chlorophyll content (Cab) and water content (Cw) were also identified as influential parameters for the visible and shortwave infrared radiation respectively. On the other hand, Hapke's soil parameters (h , $B0$ and c), dissociation factor and $LIDFb$ were recognized to have marginal influence on the output radiance. It is also found that a large portion of uncertainty in the output radiance is driven by the interaction effects among input parameters in the visible ($\sim 550nm$), whereas the red-near infrared ($\sim 670nm$), seems to be less related to the interaction effects. The results of this research support the idea of finding retrievable parameters from existing measurements of radiance using sensitivity analysis. This study has also found that generally TOA radiance sensitivities to dominant biophysical parameters are similar to BOA reflectance sensitivities provided that the visibility of the atmosphere is high (e.g. more than $23km$). This suggests that both TOA radiance images and atmospherically corrected reflectance images can be used to retrieve influential biophysical parameters of interest. However, when the visibility decreases there are some significant differences between the measured sensitivities for BOA and TOA, in particular for the visible part of the spectrum. It was also shown that the impact of viewing and illumination geometry is wavelength dependent and influences NIR and SWIR wavelengths significantly, while the observed difference between different solar/view directions was not considerable in the visible.

The proposed method requires two independent sample sets, though recent studies suggest that all first-order effects can be obtained even from a simple Monte Carlo run (Plischke et al., 2013), which would decrease computational cost noticeably. This can be considered as a further research step in developing sensitivity analysis methods for radiative transfer models if only first-order effects are demanded.

4

Multi-temporal, multi-sensor retrieval of terrestrial vegetation properties from spectral-directional radiometric data

Abstract: The synergy of a time series of optical satellite observations from a variety of sensors can be exploited to improve the retrieval of biophysical variables. Information from different sensors may assist in the variable retrieval by limiting potential ambiguities. This involves observations at different spatial, spectral, temporal and angular resolutions, etc. Furthermore, using timely data is of much importance for vegetation monitoring in environmental modeling. While the other necessary variables for such models can be collected daily (e.g. meteorological variables), the temporal resolution of optical sensors (high to intermediate spatial resolutions) does not allow having temporally frequent products of vegetation characteristics due to the revisit time of the sensors and cloud coverage. A multi-temporal, multi-sensor approach applied to a temporal sequence of radiometric data acquired by different sensors can improve mapping and monitoring of vegetation state variables over time. Even when no observations are available due to cloudiness or orbital configuration, the prior retrievals are taken.

The study provides a prototype proof of concept for a multi-temporal, multi-sensor approach to retrieve vegetation state variables using data collected by different imaging

Chapter 4 is based on:

Mousivand, A., Menenti, M., Gorte, B., & Verhoef, W. (2015). Multi-temporal, multi-sensor retrieval of terrestrial vegetation properties from spectral-directional radiometric data. *Remote Sensing of Environment*, 158, 311-330

spectral-radiometers over time. Focus is given to the retrieval of LAI, fCover and chlorophyll content over the agricultural test site in Barrax, Spain. The approach is evaluated over a limited number of remotely sensed data acquired during a short period in the Sentinel-3 Experiment (SEN3EXP 2009) field campaign. A variety of satellite observations including CHRIS-Proba, Landsat TM and ASTER are integrated and combined by means of the multi-temporal, multi-sensor approach and through inversion of a coupled surface-atmosphere radiative transfer model. We applied the iterative Bayesian model inversion in which retrievals of the current observation are incorporated as prior information to the successor observation.

This paper presents an overview of the results and challenges in utilizing the multi-temporal, multi-sensor approach and the Bayesian inversion technique in the retrieval of terrestrial vegetation properties. Overall, the accuracy obtained with data acquired by multiple sensors over time was higher than when using a single sensor. LAI and fCover were retrieved with RMSE = 0.7 (m^2/m^2) and 0.1 respectively (multiple sensors), while RMSE = 1.09 (m^2/m^2) and 0.15 respectively, when using data acquired by a single sensor.

4.1. Introduction

Land and surface biophysical characteristics are essential for understanding the Earth's terrestrial systems and for modeling the exchanges of energy and mass of carbon, oxygen and water between the earth and the atmosphere (Sellers et al., 1997). Leaf area index (*LAI*), fractional cover (*fCover*) and chlorophyll content are among the most important canopy state variables characterizing energy absorption capacity of the vegetation canopy and therefore play a crucial role in most global models of climate, hydrology, ecology and agro-ecosystem (Baret et al., 2007; Fang et al., 2003; Myneni et al., 2002).

Remote sensing has proven its potential as a unique tool for retrieving vegetation properties at both local and global scales (Gobron and Verstraete, 1997; Goel, 1988; Sellers et al., 1997; Verstraete et al., 1996). Comprehensive reviews of retrieval techniques can be found in Goel (1989), Kimes (2000), Liang (2004) and Baret and Buis (2008). In general, the approaches can be grouped into two main categories based on whether the focus is on the variables of interest to be retrieved (variable-driven approach) or on the radiometric data (radiometric data-driven approach) (Baret and Buis, 2008). A variable-driven approach requires a calibration step where a parametric model, representing the inverse model, is trained through a learning dataset. The solution is found by minimizing the distance between the variables retrieved from the inverse model and those from the training data set. To generate the learning data set, either experimental data or a model of radiative transfer can be used. Several techniques, including regression-based methods (most often linear and nonlinear regression equations between vegetation indices and variables of interest), Gaussian process (Verrelst et al., 2013a), support vector machines (Durbha et al., 2007), Artificial Neural Network (ANN) and Projection Pursuit can be used to construct the inverse model (Duveiller et al., 2011). Among them, ANN models have been recently given more attention in biophysical variable retrieval (Bacour et al., 2006; Baret et al., 2007; Fang and Liang, 2005; Liang, 2004; Schlerf and Atzberger, 2006), due to their capability to deal with multivariate and complicated problems (Duveiller et al., 2011). In a radiometric data-driven approach, the objective is to obtain the estimate that minimizes the residuals between measured and modeled radiometric data. The approach does not require calibration step, but its performance is affected by the minimization algorithm and the level of ill-posedness of the inverse problem (Baret and Buis, 2008). A number of minimization techniques have been used for implementing radiometric data-driven approaches including iterative optimization methods (Bicheron and Leroy, 1999; Jacquemoud et al., 2000; Laurent et al., 2013; Vuolo et al., 2008), genetic algorithms (Fang et al., 2003), look up tables (Hedley et al., 2009; Laurent et al., 2011a) and Monte Carlo Markov Chains (Zhang et al., 2005). Among them iterative optimization techniques and look up tables have been the most widely used in the literature (Baret and Buis, 2008).

Over the last decades, an enormous amount of work has been devoted to the retrieval of vegetation characteristics. Several satellite missions are currently being used to quantify such characteristics in a wide range of spatial and temporal resolutions and new ones are expected to become available in the coming years (with an unprecedented capacity to measure vegetation properties). Most of the satellite vegetation products are sensor-specific and rely on using measurements from a single sensor. Furthermore, using timely data is of much importance for vegetation monitoring in environmental model-

ing. While the other necessary factors for such models can be collected daily (like meteorological variables), the temporal resolution of available optical sensors does not allow for frequent updates of vegetation characteristics due to the revisit time of the sensors and cloud coverage. Platforms acquiring optical data at high or intermediate spatial resolutions (1m–100m) have a nominal revisit frequency of about a few days to a few weeks, which becomes significantly lower because of clouds. A multi-temporal, multi-sensor approach that exploits heterogeneous temporal sequences is able to retrieve vegetation properties through the subsequent updates of initial retrievals.

Moreover, due to uncertainties related to satellite measurements and radiative transfer models, as well as the limited number of independent measurements provided by a single sensor (considering the large number of variables and parameters determining spectral radiance), the retrieval problem is underdetermined and ill-posed. The ill-posedness can be effectively alleviated by regularization schemes such as the incorporation of prior information (Combal et al., 2002) taken either from ground measurements or products provided by another sensor, imposing spatial constraints (Atzberger, 2004), temporal constraints (Koetz et al., 2005) and reducing the number of free parameters (Dorigo et al., 2007). Hence, a reliable retrieval is only possible if additional assumptions, constraints or further independent observations are introduced (Combal et al., 2002; Kimes, 2000). A temporal sequence constructed through the combination of data acquired by different sensors over time is expected to help address this problem. The differences in the spectral and angular sampling, spectral sensitivity, temporal and spatial resolutions of different sensors potentially offer a source of complementary information for variable retrieval. Furthermore, a set of sensor data types with different sensitivities to vegetation properties would lead to more accurate results than those from any single sensor data type (Knyazikhin and Martonchik, 1998). Therefore, a multi-temporal, multi-sensor approach can be more successful than a single sensor in providing the user community with a range of products that can be assimilated, for instance, in crop growth models with better accuracy and more frequent products (Verhoef, 2007). Besides, a multi-temporal, multi-sensor approach for optical imageries could contribute to making unified products instead of a catalog of sensor-dependent products (Samain et al., 2006). We shall hereafter call the approach only multi-sensor for the sake of brevity.

The multi-sensor approach, based on the use of physically-based model inversion, allows the combined use of a diversity of sensors with different sensor characteristics. This helps not only to mitigate the problem of ill-posedness by providing more information from different sources but it also allows the simultaneous retrieval of multiple variables and parameters. The multi-sensor variable retrieval can also improve the continuity of the biophysical variable maps over time for a region of interest. Even when no observations are available due to cloudiness or the orbital configuration, the prior retrievals are taken.

A number of studies have already pointed out the potential of a multi-sensor approach to improve the reliability and consistency of vegetation state variables. State variables can be defined as the main variables governing radiative transfer processes within the canopy (Verstraete et al., 1996). For instance; combining multi-temporal data from identical sensor (Hagolle et al., 2005; Koetz et al., 2007; Lauvernet et al., 2008; Menenti et al., 2005; Yang et al., 2006), synthetic data (Verhoef, 2007), a synergy of LIDAR data with

spectral measurements (Koetz, 2006), combining hyperspectral and synthetic aperture radar (Treuhaft et al., 2002, 2004), integrating spectral and directional measurements (D'Urso et al., 2004; Widlowski et al., 2004) and a synergy of an ensemble of imaging instruments (Geiger et al., 2004; Jin et al., 2002; Samain et al., 2006). Although the retrieval of vegetation state variables from these multi-sensor approaches represents a promising advance in improving the quality of the retrieved products, the differences in sensor characteristics (spectral, radiometric, spatial and angular) and acquisition geometry pose a number of challenges for the implementation of such an approach. We will discuss these challenges in detail in the following sections.

We may distinguish two general approaches to the concept of multi-sensor variable retrieval. One is based on defining a standard framework (sensor) and normalize all the radiometric data by that framework (Samain et al., 2006), then performing the retrieval on the normalized data. The other approach is based on the simulation of reflectance/radiance for each sensor independently using RT models and integrate such simulations for variable retrieval. The former approach requires defining a sensor as the reference to which the other measurements are converted. This phase, in turn, consists of various steps in data preprocessing and correction (e.g. spectral and angular normalization) to match the measurements with different scales and resolutions to the reference configuration. Instead, we consider the latter approach that requires no normalization on the data, provided that the satellite images are geometrically corrected and resampled to a common pixel size. Model inversion of at-sensor radiance by forward model simulation has the advantage that no correction/conversion is necessary and raw radiance data can be used for inversion.

The multi-sensor variable retrieval may be performed using either Top-Of-Canopy (TOC) reflectance or Top-Of-Atmosphere (TOA) radiance. In the former case, prior to retrieval procedure, preprocessing and corrections have to be done on satellite imagery to transform what has been recorded by a sensor into TOC reflectance. This involves a series of corrections such as atmospheric correction, angular effects and topographic (illumination) corrections. Such corrections are often done separately in a sequence and commonly independent of one another. In addition to error propagation caused by these corrections, due to the inter-related effects of the atmosphere and the surface, independent processing would not reflect the physical interaction of the system (Laurent et al., 2011a). Therefore, the multi-sensor approach requires careful modeling of sensor radiance. In this way we directly simulate TOA radiance for each sensor and the retrieval is performed at sensor level (i.e. radiance at-sensor). The TOA radiance is simulated using the coupled Soil-Leaf-Canopy model SLC and MODTRAN4 RT model (Verhoef and Bach, 2003b, 2007, 2012). Coupling surface-atmosphere RT models would also allow retrieving atmospheric properties and surface properties simultaneously in case spectral radiance is measured at wavelengths sensitive to those properties.

The inversion algorithm used in the multi-sensor approach has to be effective to invert highly non-linear RT models against satellite measurements, not only in finding a global minimum of the cost function at low computational cost (i.e. fast convergence), but also to incorporate a priori information about the solution into the retrieval (Dorigo et al., 2007; Verhoef, 2007). In our study, this prior information comes from the retrievals of the previous observation (image data). Look-Up Table (LUT) and machine

learning techniques (e.g. neural networks) have been frequently and successfully applied in biophysical variable retrieval. The LUT technique is very simple, yet suitable to find a rough global minimum of the cost function. Machine learning methods are also among robust computationally efficient methods in variable retrieval. However, in the multi-sensor approach a number of sensors with different characteristics (e.g. illumination/observation geometries) plus large number of spectral bands are incorporated. With such a high dimensionality, model inversion approaches such as machine learning methods and LUT techniques tend to become less practical and iterative optimization methods re-emerge as a feasible alternative. Bayesian model inversion is a promising way to accomplish this task since it allows the incorporation of prior information about the solution into the retrieval. This is indeed important in the multi-sensor approach where the retrievals from previous measurements can be incorporated into the retrieval procedure with the new measurements.

In the here presented multi-temporal, multi-sensor approach, the surface properties are stored in a geo-database (e.g. a Geographic Information System (GIS)) and an updating rule is used to constrain the degree of belief in stored information versus new observations over time. When a new observation is assimilated, prior to the inversion, the dimensionality of the dataset is exploited and then a sensitivity analysis is performed to identify retrievable variables given the available measurements. This also helps to avoid the inversion to become ill-posed. Then, the Bayesian model inversion is applied using both radiometric data and prior information (taken from the geo-database) to update relevant surface properties. Sensor radiometric performance and prior information are used to attach weights to the radiometric data and to the various variables.

The overall objective of this work is to investigate the use of the multi-temporal, multi-sensor approach to retrieve vegetation state variables through physically-based Bayesian model inversion of a coupled surface-atmosphere radiative transfer model. The focus is on the retrieval of LAI, fCover and chlorophyll content over the agricultural test site in Barrax. The data set considered in the study was acquired during the Sentinel-3 Experiment (SEN3EXP 2009) field campaign sponsored by the European Space Agency (ESA). A number of satellite sensors including CHRIS-Proba, Landsat and ASTER have been used in the multi-sensor framework. The remainder of the paper is organized as follows. Section 4.2 describes the ground measurements and the satellite observations collected during the field campaign. In Section 4.3, the methodology is given and different aspects of the multi-temporal, multi-sensor approach including an extensive discussion on Bayesian model inversion and relevant issues are discussed. Section 4.4 presents the results obtained from different scenarios considered in the study. Section 4.5 is devoted to the discussions and in Section 4.6 we draw the conclusions of the work.

4.2. Material and methods

4.2.1. Field ground measurements

For the application of the multi-temporal, multi-sensor approach, observations and ground truth measurements acquired during the ESA SEN3EXP field campaign were used. The field campaign was carried out at the Barrax (N39°3', W2°60') test site and

surrounding area from 20 to 24th of June 2009 as part of the development process for ESA's Sentinel-3 Earth observation mission (Brockmann et al., 2011). The SEN3EXP data was chosen due to the number of available observations and also the time span of the field campaign. Barrax is an agricultural test site located in southeastern Spain on the La Mancha plateau. The area is characterized by large uniform agricultural fields and consists of approximately 65% rain-fed and 35% irrigated crops. The area has been sampled in several field campaigns for many years because of its flat topography (with differences in elevation ranging up to only 2 m) and large crop fields with some fields measuring 1 km in diameter, offering appropriate targets for these studies. Agriculture mainly concentrates on irrigated alfalfa, corn, onion, oat, garlic, potato, sunflower and rain-fed crops such as barley and wheat. Figure 4.1 illustrates the distribution of different crops during the field campaign. Wheat and barley fields were senescent at the time of the field campaign and many fields were already harvested. Not-irrigated fields such as bare soil, fallow and already harvested fields were covered by vegetation not characterized by the data collected during the campaign. Accordingly, such fields were masked out according to the landuse/landcover map provided in the campaign dataset and they are not included in our analysis. Among the irrigated crops, corn and sunflower fields were at different stages of development (ranging between 0.5 and 1.5 meters height). Other crops were onion, garlic, potato and oat and some crop types in minor proportion (e.g., vineyard, fruit trees, papaver).

Different vegetation properties including chlorophyll, LAI, FAPAR, fCover, EWT, structural parameters, leaf transmittance and reflectance were collected concurrently with the satellite observations. The following crops were sampled: alfalfa, barley, bare soil, corn, festuca, fruit, garlic, oat, potato, sunflower, vine and wheat. The dry soil reflectance spectra were obtained by an ASD spectro-radiometer during the campaign. The atmospheric visibilities and water vapor columns were also measured concurrent with the satellite overpass. The study area (Figure 4.1 dashed white line) was chosen to include most of the sampled ground points subject to satellite coverage, covering an area of around 2500 hectares. A total of 43 elementary sampling units (ESUs) were characterized within our study area corresponding to 12 different fields of 8 vegetation types. However, there were no LAI and fCover measurements for four ESUs, including three oat and one alfalfa samples, in the campaign dataset and only 38 ESUs had chlorophyll content measurements.

4.2.2. Earth observation data

A number of satellite observations were acquired concurrently with ground measurements of vegetation properties at the Barrax during the SEN3EXP campaign (Brockmann et al., 2011). Spectral-radiometric data collected by three different sensors were used for the current study. Two hyperspectral and multi-angular CHRIS-Proba datasets (Compact High Resolution Imaging Spectrometer), two Landsat TM images and an ASTER image were used.

A primary full ASTER dataset consists of 15 spectral bands: three basic bands in the visible and near infrared (VNIR) with a 15m resolution plus one VNIR which points backwards to create a stereo view, six bands in the short wave (SWIR) with a 30m resolution and five thermal bands (TIR) with a 90m resolution. The ASTER image was captured on

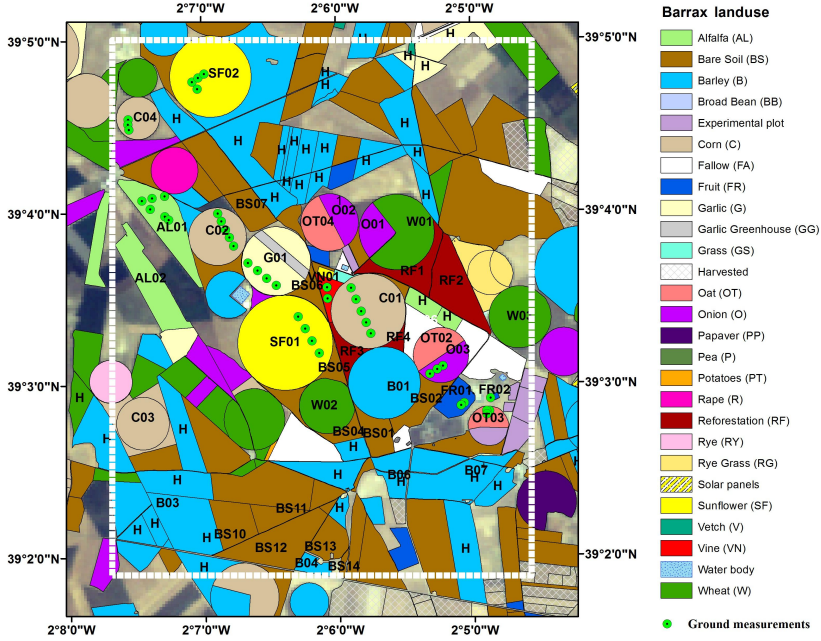


Figure 4.1: Study area Barrax during the campaign SEN3EXP 2009, sample points (green dots) and the study area (dashed white line). The harvested fields are labeled with “H”. Green dots represent sample points where LAI, fCover and Cab were measured. The oat field includes only Cab measurements and no LAI, fCover measurements were available for this field. A total of 40 elementary sampling units (ESUs) were characterized within our study area corresponding to 12 different fields of 8 vegetation types

21 June 2009 during SEN3EXP campaign which was the ASTER L1B (registered radiance at sensor product). The image was geometrically corrected with an accuracy of approximately 0.1 pixel for VNIR spectral bands. As of April 2008 the ASTER SWIR detectors no longer functioned. Therefore, we have used the three visible bands in our analysis.

The CHRIS-Proba datasets were acquired on 19th and 20nd June 2009 in Mode-1 (agriculture mode) with 62 spectral bands from 372 nm to 1036 nm with a nadir ground sampling distance of 34m spatial resolution. The CHRIS instrument provides hyper-spectral data at five different viewing angles with nominal fly-by zenith angles (FZAs) at $\pm 36^\circ$, $\pm 55^\circ$ and 0° (nadir) quasi-simultaneously (Barnsley et al., 2004). Figure 4.2 illustrates the angular sampling of the two CHRIS-Proba datasets. We have used all the CHRIS-Proba images (i.e. all view angles) on June 19th in our analysis. Unfortunately, the forward-looking 55° view zenith angle image on June 20th was not correctly acquired and the backward-looking 55° view zenith angle image was very noisy. Therefore, on June 20th only three images (-36° , nadir and $+36^\circ$) were included in our analysis. The preprocessing of the TOA radiance CHRIS datasets including noise reduction (i.e. correcting drop-outs and destriping) was done with the open source software BEAM (CHRIS-ToolBox) (WWW, a). The CHRIS datasets were then geometrically corrected using 15 to 20 ground control points (depending on the viewing angle) extracted from the

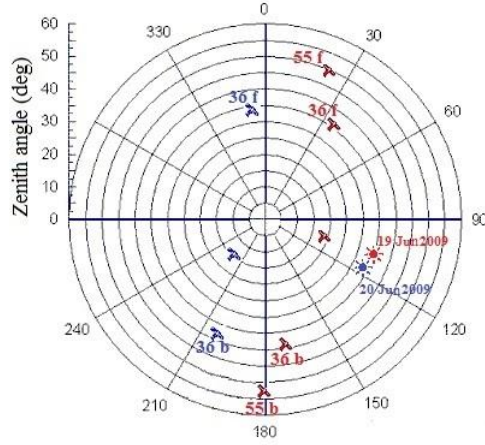


Figure 4.2: Angular sampling of the two CHRIS-Proba images on 19th June (red) and 20th June 2009 (blue). Labels are nominal zenith angles “f” stands for forward looking and “b” represents backward looking

ASTER image (15m spatial resolution). The Root Mean Square Error (RMSE) was less than one pixel for all the angles (not shown) indicating a reasonable spatial accuracy. The error was generally smaller for nadir and increased with the view angle.

Two TOA radiance Landsat images (TM) with 30m resolution on 13th and 22nd June 2009 were downloaded from the United States Geological Survey (USGS) website. The Landsat images were geometrically corrected with an accuracy of 0.19 and 0.17 pixels for the images on 13th and 22nd June, respectively. The scaled TOA radiance was transformed to actual radiance with the information provided in the header-files. In the multi-temporal, multi-sensor approach all image data are resampled to the same reference grid using nearest neighbor technique. We have chosen 30m since it applies to both TM and ASTER images. No atmospheric correction was done on the datasets and a set of co-registered and geo-referenced images, containing the TOA spectral and angular radiance were ultimately used for the retrieval.

4.2.3. Top Of Atmosphere (TOA) radiance

The spectral radiance recorded by a sensor is the integrated sum of several components including surface reflectance, atmospheric effects and target's surroundings convolved with the sensor spectral and spatial response functions. The four-stream radiative transfer theory proposed by Verhoef and Bach (2003b, 2007, 2012) can effectively model this integration. Consistent with the notations adopted by Verhoef and Bach (2003b), we represent TOA radiance as;

$$L_{TOA} = \frac{E_s^0 \cos(\theta_s)}{\pi} \left[\rho_{so} + \frac{\tau_{ss}\overline{r_{sd}} + \tau_{sd}\overline{r_{dd}}}{1 - \overline{r_{dd}}\rho_{dd}} \tau_{do} + \tau_{ss}r_{so}\tau_{oo} + \frac{\tau_{sd} + \tau_{ss}\overline{r_{sd}}\rho_{dd}}{1 - \overline{r_{dd}}\rho_{dd}} r_{do}\tau_{oo} \right] \quad (4.1)$$

The definitions are given in Table 4.1; the over bars in Eq 4.1 indicate spatial aver-

aging over the surroundings of the target to account for the adjacency effect. According to Eq 4.1, four surface reflectance factors plus six atmospheric coefficients are needed in the four-stream approach to simulate TOA radiance (see Table 4.1). The surface reflectance components are modeled by the SLC RT model and the atmospheric coefficients are extracted from the MODTRAN4 atmospheric model. Eq 4.1 is simplified by neglecting the adjacency effect in the simulations due to difficulties in the calculation of this effect for pixel-wise model inversion. The SLC and the MODTRAN4 models are described in the following sections.

4.2.3.1. Soil-Leaf-Canopy (SLC) RT model

The top-of-canopy reflectance signatures are modeled by the integrated Soil-Leaf-Canopy RT model SLC (Verhoef and Bach, 2007). The reflectance signature in SLC is a function of structural and optical properties of soil, leaf, and canopy and of the illumination and viewing geometry. SLC simulates reflectance spectra over the spectral range between 400 and 2500 nm for arbitrary sun-target-sensor geometries. SLC relies on a four-stream extended version of the SAIL radiative transfer model (Verhoef, 1984), which uses four radiance fluxes: direct solar flux, diffuse downward flux, diffuse upward flux and directly observed flux. The outputs of the model are four directional reflectance factors of the canopy plus two canopy absorptances (Verhoef and Bach, 2007). The four canopy reflectances are r_{so} , r_{do} , r_{sd} and r_{dd} in Table 4.1 and the two canopy absorptances are for direct solar incident flux and for hemispherical diffuse irradiance.

Table 4.1: Terminology used in the study (after Verhoef and Bach (2003b, 2007, 2012))

Variable	Description	RT model
L_{TOA}	TOA radiance	-
r_{so}	Surface bidirectional reflectance	SLC
r_{do}	Surface hemispherical-directional reflectance	SLC
r_{sd}	Surface directional-hemispherical reflectance	SLC
r_{dd}	Surface bi-hemispherical reflectance	SLC
ρ_{so}	TOA atmospheric bidirectional reflectance	MODTRAN
ρ_{dd}	Bottom Of Atmosphere (BOA) spherical albedo of the atmosphere	MODTRAN
τ_{ss}	Direct atmospheric transmittance from the sun to the ground	MODTRAN
τ_{oo}	Direct atmospheric transmittance from the ground to the sensor	MODTRAN
τ_{sd}	Diffuse atmospheric transmittance from the sun to the ground	MODTRAN
τ_{do}	Diffuse atmospheric transmittance from the ground to the sensor	MODTRAN
E_s^o	Extraterrestrial solar irradiance on a plane perpendicular to the sunrays	-
θ_s	Local solar zenith angle	-

To simulate soil reflectance and its variability with moisture, unlike its predecessors, SLC treats the soil background as an anisotropic reflector where a non-Lambertian extended version of Hapke's soil BRDF model (Hapke, 1981) containing the hotspot and soil moisture (SM) effects has been incorporated. Two different types of leaves (green and brown) are considered in SLC. The transmittance and reflectance of leaves is modeled by an extended version of the PROSPECT leaf reflectance model (Jacquemoud and Baret, 1990) that considers brown pigments (Verhoef and Bach, 2003a). The PROSPECT model takes five variables as input; leaf internal structure variable (N), leaf chlorophyll

content (Cab), leaf dry matter content (Cdm), leaf water thickness (Cw) and leaf brown pigment (Cbrown) (Jacquemoud and Baret, 1990; Verhoef and Bach, 2003b). Using the brown pigment variable is useful to discriminate photosynthetic and non-photosynthetic light absorption components.

The 4SAIL2 model (Verhoef and Bach, 2007) is employed to simulate the canopy as a two-layer structure where a crown clumping effect (as in forests) is taken into account. The clumping effect is described by two additional parameters; vertical crown coverage (Cv) and tree shape-factor (Zeta). The latter is equal to the ratio of crown diameter to crown height. The Leaf Inclination Distribution Function (LIDF) is modeled by two parameters: LIDF parameter a (LIDFa), which controls the average leaf slope and LIDF parameter b (LIDFb), which controls the so-called distribution's bimodality (Verhoef and Bach, 2007). Both, LIDFa and LIDFb can vary between -1 and 1, but the sum of their absolute values must be always less than or equal to 1. In 4SAIL2, the LIDF parameters are assumed to be identical for both layers, as well as the size parameter of the hot spot effect (Hot). The ratio of leaf width to canopy height can be considered as an estimate of the hot spot magnitude which is strongly related to the sharpness of the hot spot peak. Furthermore, two parameters are used to characterize the mixture of green and brown leaves in the canopy, namely the fraction of brown leaf area (FB) and a dissociation factor (Diss). When all green leaves are in the top layer and all brown leaves are laid down in the bottom layer, the dissociation factor is equal to 1. In case of dissociation equal to zero, all leaves are homogeneously mixed over the two layers. The variable fCover, which is considered as one of the retrievable state variables, is actually an output of the SLC model rather than an input. It is one minus the direct transmittance of the canopy layer after consideration of clumping by tree crowns. The effective cover becomes

$$fCover = Cv \left(1 - e^{-k \cdot LAI} \right) \quad (4.2)$$

Here k is the extinction coefficient in the vertical direction (related to LIDF parameters) and Cv is the vertically projected crown cover fraction. The suitability of different versions of the PROSPECT-SAIL model to simulate top of canopy reflectance has been demonstrated in many studies (Atzberger and Richter, 2012; Bach and Verhoef, 2003; Huemmrich, 2001; Jacquemoud et al., 2009; Major et al., 1992; Meroni et al., 2004). The 4SAIL2 model accuracy has also been verified by comparison against other models in the RAMI project (Widlowski et al., 2007) and with satellite and ground measurements (Verhoef and Bach, 2007). In the RAMI-3, the 4SAIL2 is shown to be in good agreement with the ensemble of all other models with less than 4% difference in BRDF simulations. Verhoef and Bach (2007) have demonstrated that the SLC model was fitted to CHRIS-Proba data of the Upper Rhine Valley in Germany for different types of vegetations and bare soil with an average RMS error of 1.6% for nadir viewing, 2.34% for $\pm 36^\circ$ and 3.3% for oblique observations with $\pm 55^\circ$ between measured and simulated reflectances. The TOA radiance simulation using the four-stream approach and the coupled SLC-MODTRAN4 has been utilized for model inversion (Laurent et al., 2011a,b) and sensitivity analysis (Mousivand et al., 2014). The top-of-canopy reflectance factors simulated by SLC are combined with the atmospheric coefficients calculated with MODTRAN4 to obtain the TOA spectral-directional radiance.

4.2.3.2. MODTRAN (MODERate resolution TRANsmittance and radiance code)

MODTRAN4 is a radiative transfer code developed initially from the LOW resolution TRANsmittance 7 (LOWTRAN 7) model. The code is a state-of-the-art radiative transfer code and models scattering and absorption effects in the atmosphere with high accuracy and high spectral resolution up to 1 cm^{-1} in wavenumber units. The scaled DISORT (DIScrete Ordinate Radiative Transfer) algorithm is integrated for accurate computations of atmospheric multiple scattering and the correlated k algorithm is applied for the spectral regions with significant absorption effects (Berk et al., 1998). All these features make MODTRAN4 a good candidate for realistic simulation and analysis of remote sensing measurements. MODTRAN4 is well-suited for both at sensor radiance simulation (Guanter and Kaufmann, 2009; Laurent et al., 2011a; Schlapfer and Nieke, 2005; Verhoef and Bach, 2007, 2012) and for atmospheric correction (Adler et al., 1999; Schlapfer and Richter, 2002) from the ultra-violet to the thermal infrared wavelengths.

The computational burden of a MODTRAN4 run depends strongly on the calculation mode and also whether applying DISORT with various radiative streams. In the four-stream approach, the six atmospheric coefficients in Eq 4.1 can be obtained with three MODTRAN4 runs for surface albedos at 0, 0.5 and 1(–). We have modified the algebra used by Verhoef and Bach (2003b, 2007) to make it more computationally efficient and also to avoid using zero albedo since it leads to some miscalculations in the extracted coefficients from MODTRAN4 (Guanter et al., 2009). In the modified version we only need two MODTRAN4 runs for surface albedos at 0.5 and 1(–) to derive all the six atmospheric coefficients. The direct use of the MODTRAN4 code in inverse modeling is not practical because of the computational limitations. Therefore, we have generated a large 6-tuple look-up table filled with the six atmospheric coefficients from a series of MODTRAN4 runs. The free parameters were wavelength (2101 wavelengths), water vapor (4 values), visibility (5 values), relative azimuth angle (5 values), solar zenith angle (7 values) and view zenith angle (7 values) with the purpose of covering a large number of atmospheric profiles. Linear interpolation between LUT entries is used for forward simulation of TOA radiance during model inversion avoiding direct calls to the MODTRAN4 code. The LUT may also be used to retrieve atmospheric parameters such as visibility and water vapor content by model inversion. The TOA radiance simulations were performed at intervals of 1 nm and these simulations were later convolved with the relevant sensor spectral response functions in order to produce sensor-like radiometric data.

4.3. Methodology

The scheme in Figure 4.3 shows how the multi-temporal, multi-sensor approach is applied to retrieve biophysical variables using data collected by various satellite sensors over time. The multi-temporal, multi-sensor is designed for the exploitation of a temporal sequence constructed by combining data acquired by different sensors over time. The surface properties are stored in a geo-database where target properties are updated by means of satellite observations. The geo-database contains maps of all the SLC inputs (23 inputs) over the study area plus ancillary information such as metadata of different maps, atmospheric parameters and covariance matrices. The architecture and format of the geo-database is similar to an “*ArcGIS File Geodatabase*”. When a new observation is acquired, first, the dimensionality of data is explored and a sensitivity analysis is per-

formed to identify the retrievable variables given the characteristics of the sensor. Second, the TOA radiance simulated by the coupled surface–atmosphere SLC–MODTRAN4 RT model, adapted to the spatial, spectral and geometric configuration of the sensor, is compared to the measured radiance through the iterative Bayesian model inversion (Figure 4.4).

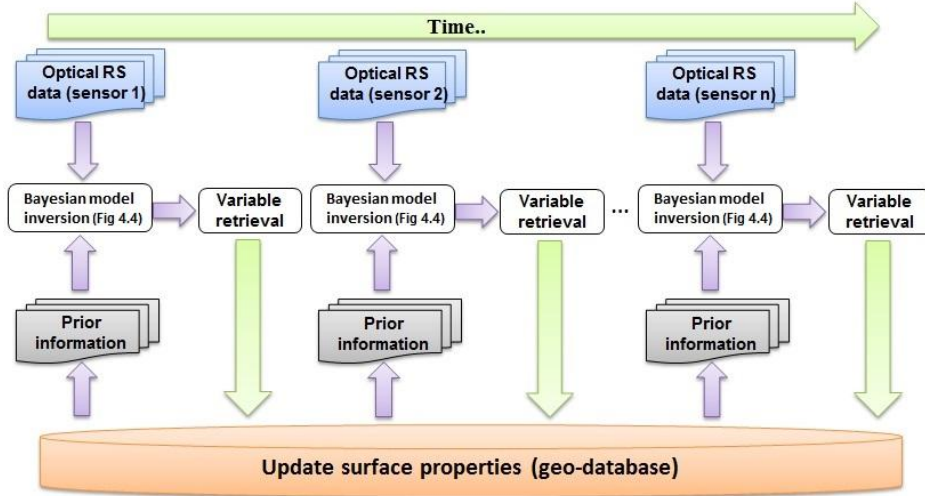


Figure 4.3: Multi-temporal, multi-sensor variable updating methodology by balancing new observation data with existing prior information

The cost function (see Eq 4.8) to be minimized consists of both a radiometric term (i.e. the difference between the simulated and the measured radiances) and a priori information term (the distance between the new retrievals and the a priori retrievals). Comparison of both radiances leads to the adjustment of surface properties and these are then fed back until measured and simulated radiances match best and the cost function reaches its minimum. In the Bayesian model inversion, the uncertainties in the state variables and measurements are directly incorporated in the analysis. Moreover, the uncertainties of the retrievals are provided by the Bayesian inference as an output. The uncertainties are represented as (co)variance matrices to weigh the a priori information for the next scheduled observation. We shall in the following sections discuss different aspects of the multi-sensor approach.

4.3.1. Dimensionality and sensitivity analysis

The number of biophysical variables to be retrieved through inversion of a radiative transfer model is limited by the number of independent measurements of radiance (Goel, 1988; Kimes, 2000; Menenti et al., 2005). Even in the case of hyperspectral and multi-angular observations, the number of independent (i.e. non-correlated) measurements is often far smaller than the number of spectral bands. The computational and statistical efficiency of retrieval techniques degrade rapidly with the dimensionality of the dataset

(this phenomenon is often referred to as the “*curse of dimensionality*”). A requirement for meaningful variable retrieval is to find out how many variables are needed to represent the spectral radiance, which is known as the so-called “*intrinsic dimensionality*”. Estimating the intrinsic dimensionality of a dataset would give an estimate of the number of independent measurements which in turn indicates the maximum feasible number of free variables during inversion.

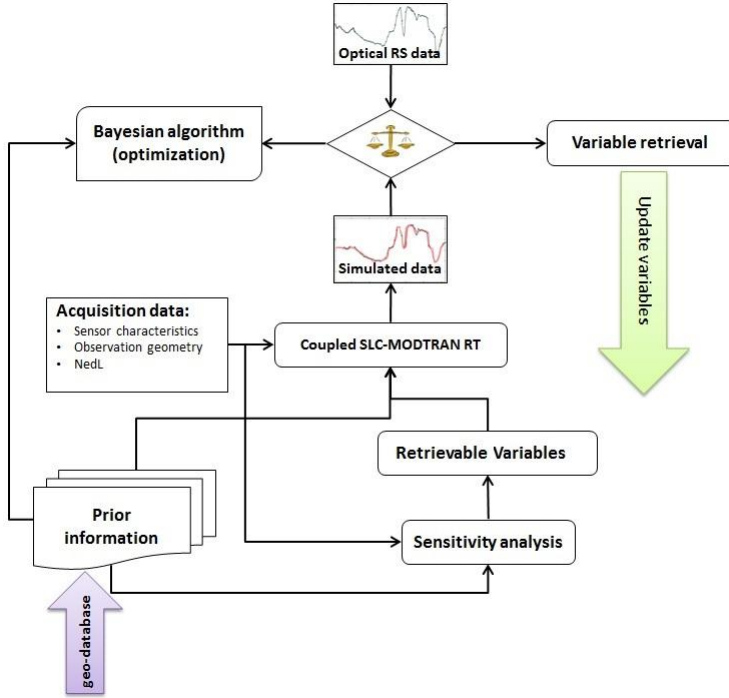


Figure 4.4: Iterative Bayesian model inversion in the variable retrieval approach

A number of methods have been proposed for estimating the intrinsic dimensionality of a dataset. Among other methods, Principal Component Analysis (PCA) is a popular technique to determine the intrinsic dimensionality which makes use of the eigenvalue distribution (Bouveyron et al., 2011; Theodoridis and Koutroumbas, 2009). We have performed principal component analysis on vegetated areas to estimate the intrinsic dimensionality of different data sets. The eigenvalues of the covariance matrix of a multivariate dataset are an indication of the shape of the subspace where the data is embedded. The intrinsic dimension can be determined as the number of eigenvalues greater than a given threshold (Settle, 2004). To determine the threshold, the empirical indicator function proposed by (Malinowski, 1977) was used. Note that the intrinsic dimensionality estimated by such a method is an upper bound on the true intrinsic dimensionality (Chang and Du, 2004). Therefore, we subtract one from the estimated value to avoid overestimation and get more consistent results on the intrinsic dimensionality.

Once the intrinsic dimensionality of the dataset has been found, it is important to

explore which variables are the most influential and retrievable on the existing measurements of radiance. Retrievable variables are those physical quantities to which the measurements are sensitive. In this special case of the coupled SLC–MODTRAN4 model, there are 23 surface–atmosphere model variables, which can be simultaneously retrieved. However, this number is far beyond what can be retrieved in reality, because of the number of independent observations required. This means that only the most influential variables should be included in the inversion.

Sensitivity analysis is able to identify the most influential variables by forward modeling (Mousivand et al., 2014). This determines the variables that can be updated by the given observation and for which variables a fixed value may be used during inversion. In an ideal case, the necessary and sufficient condition for a model variable to be non-influential is that the main effect and the interaction effects with other variables are zero, which shows that the contribution of the variable on the output variance is zero. This condition allows assigning an arbitrary value to that variable within its domain. In practice, model variables can be treated as non-influential if their effect on the radiance at a given wavelength is very small compared to the other variables. A non-influential variable cannot be retrieved with the given measurements (Mousivand et al., 2014). As shown in Figure 4.4, sensitivity analysis is performed prior to the inversion of each new image data set. The analysis of the sensitivity of TOA spectral radiance to model variables is carried out using the winding stairs sensitivity analysis method proposed by Mousivand et al. (2014). This is a global sensitivity analysis method, which applies the Sobol sequence generator (Sobol, 1993) to select a number (n) of baseline points in the model variables space. The values of model variables at a baseline point are perturbed sequentially one at a time, until all model variables are perturbed once per each baseline point. The perturbation is done based on the winding stairs variation technique and for each baseline point, at the end, a block (*trajectory*) of sample points is formed within the model variables space. Sensitivity effects are then computed from n such blocks, each of size $(m + 1)$, where m is the number of model variables. Consequently, the total cost of the method is $n(m + 1)$. The method provides total-order sensitivity effects comparable with sophisticated variance-based methods with modest computational time. The ranges of the model variables are chosen based on the prior information and acquisition properties. A number of 100 trajectories in the model variables space corresponding to 2000 canopy realizations (for 19 model variables out of 23 since four soil variables were assumed fixed) were taken to perform the sensitivity analysis.

4.3.2. Bayesian model inversion

Bayesian methods for variable retrieval allow the incorporation of prior information about the solution, which might come from other data sources. In multi-sensor approach the retrieval procedure refines previous retrievals by narrowing their Probability Distribution Function (*PDF*). The prior information with the *PDF* $P(p)$ summarizes information about variable p before any data are collected. Bayes' theorem can be stated as follows.

$$P(p | L_{obs}) = \frac{P(p) P(L_{obs} | p)}{P(L_{obs})} \Rightarrow P(L_{obs}) \approx \int_{all parameters} P(p) P(L_{obs} | p) dp \quad (4.3)$$

where p is the vector of variables to be retrieved, L_{obs} is the vector of measured radiances, $P(p)$ is the *PDF* of p , $P(L_{obs} | p)$ is the conditional *PDF* of L_{obs} given p (i.e. the likelihood function), $P(p | L_{obs})$ is the conditional *PDF* of the variables to be retrieved given the observations, which is also called posterior probability of variables of interest. The posterior probability is proportional to the product of the likelihood function and the prior probability. Since in the Bayesian approach we want to maximize the posterior probability, Eq 4.3 can be written as

$$P(p | L_{obs}) \propto P(p) P(L_{obs} | p) \quad (4.4)$$

For Bayesian inference, the prior information about the variable of interest is formalized by considering it a random variable p characterized by its prior probability function $P(p)$. However, it is not vital to believe in a strict probabilistic interpretation of the prior. In many circumstances, the prior is just a (technical) way of expressing available information leading to an inference procedure. In particular, the Bayesian paradigm (formally) allows considering priors than are not normalized (nor normalizable), which are then called improper priors. The Bayesian approach brings inversion down to the determination of an a posteriori law. Since we cannot envisage calculating such laws completely, we content ourselves with looking for a point estimator, which is often the maximum a posterior. When considering parameters as random variables with a multivariate normal distribution, the joint probability density function is defined as

$$P(p) = \frac{1}{\sqrt{(2\pi)^m \det(C_p)}} \exp\left(-\frac{1}{2} (p_{prior} - p)^T C_p^{-1} (p_{prior} - p)\right) \quad (4.5)$$

where p_{prior} is the vector of expected values of p , C_p contains the covariance between variables and m is the number of free variables. In Eq 4.5, if C_p is singular, then the joint probability density function is not defined. The vector p_{prior} and the covariance matrix C_p completely characterize the multivariate distribution and have to be computed very carefully. Similarly the conditional probability distribution of observations given the current state of variables is

$$P(L_{obs} | p) = \frac{1}{\sqrt{(2\pi)^n \det(C_L)}} \exp\left(-\frac{1}{2} (L_{obs} - L_{mod})^T C_L^{-1} (L_{obs} - L_{mod})\right) \quad (4.6)$$

where n is the number of observations, L_{mod} is the vector of forward simulated radiances and C_L is the covariance matrix of the model and measurements. Thus, by substituting Eq 4.5 and Eq 4.6 into Eq 4.4 we have

$$P(p | L_{obs}) \propto e^{-\frac{1}{2} [(L_{obs} - L_{mod})^T C_L^{-1} (L_{obs} - L_{mod}) + (p_{prior} - p)^T C_p^{-1} (p_{prior} - p)]} \quad (4.7)$$

The solution can be found by minimizing the negative of the exponent in Eq 4.7

$$\min \left[(L_{obs} - L_{mod})^T C_L^{-1} (L_{obs} - L_{mod}) + (p_{prior} - p)^T C_p^{-1} (p_{prior} - p) \right] \quad (4.8)$$

The minimum of Eq 4.8 (i.e. the cost function) can be found by applying an iterative nonlinear optimization algorithm. Here, the retrieval is performed by the *Levenberg-Marquardt* method (which is a modified Gauss–Newton method with a damping factor), where the forward model is initialized as linear, according to

$$L_{obs} - L_{mod} = J(p_{prior} - p) + (higher_order_terms) \quad (4.9)$$

where the Jacobian matrix J of the partial derivatives of the model output with respect to variable changes represents the linearization of the forward model at each iterative stage. The *Levenberg-Marquardt* method is an iterative calculation that computes a new estimate for the state vector (p_{i+1}) at each iteration i using a forward–model linearization at the current state vector estimate (J_i), neglecting the subscripts for brevity, the update in each iteration is:

$$\Delta p = \left[J^T C_L^{-1} J + C_p^{-1} + \lambda \text{diag}(J^T J) \right]^{-1} \left[J^T C_L^{-1} (L_{obs} - L_{mod}) + C_p^{-1} (p_{prior} - p) \right] \quad (4.10)$$

where Δp is the change in variables required to resolve the difference ($L_{obs} - L_{mod}$) between the current model solution and the measured radiance subject to the prior term, λ is the damping factor in the *Levenberg-Marquardt* that is adjusted during the course of the algorithm to ensure convergence. One important reason for using λ (a positive value) is that the $\lambda \text{diag}(J^T J)$ term ensures that the matrix is nonsingular. Since the matrix in this system of equations is symmetric and positive definite, we can use the Cholesky factorization to solve the system. *Levenberg-Marquardt* has been originally developed for unconstrained nonlinear problems, but in our case the problem is constrained because the upper and the lower bounds of the variables are known. To limit the solution space to the set of feasible solutions, one can use a penalty function or a transformation of the state vector. We have used a transformation of the state vector into a periodic space (WWW, b) and the inversion takes place over the periodic space. If a proposed solution falls outside of the feasible region of the state vector, this transformation projects it back to the feasible region. The iteration proceeds until the convergence criteria are met or the iteration limit (100 iterations here) is reached. The convergence criteria tests the change in the state vector estimate with a limiting factor of 0.01, which means the iteration will continue until the change is smaller than this value. The initial values of the free variables were set according to values in Table 4.3. For the variables and parameters with ground truth data, these values were chosen very close to the mean of the measured values. The prior expected values and (co)variance matrix were taken from the previous retrievals (as stored in the geo-database).

The update rule in Eq 4.10 is very similar to *zeroth – order* Tikhonov regularization in the special case where the covariance matrices are diagonal (i.e. they become a variance matrix). In other words, the solution obtained by using independent and normally distributed prior variables is precisely the Tikhonov regularized solution. However, this does not mean that the Bayesian approach is entirely equivalent to Tikhonov regularization, since the Bayesian solution is a probability distribution, whereas the Tikhonov solution is a single point estimation. With linearization around the optimal solution, we can obtain the approximate posterior covariance from the curvature of the cost function

at its optimal solution which is the inverse of the Hessian matrix (i.e. the second order derivatives). When the residuals are very small at the solution, the posterior covariance is:

$$C_{posterior} = [J^T C_L^{-1} J + C_p^{-1}]^{-1} \quad (4.11)$$

It is worth considering what happens to the posterior distribution in the extreme case in which the prior distribution provides essentially no information. Consider a prior distribution with a covariance matrix $C_p = \alpha^2 I$ in the limit where α is extremely large. In this case, the diagonal elements of C_p^{-1} will be extremely small, and the update rule will be approximated by

$$\Delta p = [J^T C_L^{-1} J + \lambda \text{diag}(J^T J)]^{-1} [J^T C_L^{-1} (L_{obs} - L_{mod})] \quad (4.12)$$

Likewise, when there is no observation, the a priori solution is taken. The success of knowledge-based Bayesian inversion is strongly dependent on the accumulation of the uncertainties in a priori knowledge, forward model and instrument model. We will discuss each uncertainty component in further detail.

4.3.3. Prior covariance matrix

To obtain an accurate posterior distribution, we have to make realistic assumptions on the prior distribution. These assumptions are inherently subject to uncertainty with a priori knowledge which is represented by the covariance matrix. This requires accurate estimation of the covariance matrix of a priori knowledge. However, this is not a trivial task since in many cases no adequate information exists about the variable distributions or this information is vaguely defined as lower and upper bounds for the variables. In the multi-temporal, multi-sensor approach we can overcome this problem with the information provided by the predecessor observations of the variables of interest. In the case of first observation, only radiometric data are used in the inversion. After that, the posterior covariance matrix of retrievals plays the role of the a priori covariance matrix for the successor retrieval. Such covariance matrices are stored in the updated geo-database pixel-wise and when a new observation becomes available these covariance matrices are used to weight the a priori term in the cost function.

Depending on temporal auto-correlation between observations (i.e. images), some elements of covariance matrix C_p may be considered steady over a short period of time (e.g. Cab, N), however some other like soil moisture and atmospheric properties (in case they are treated as free variables) vary rapidly with time from one observation to another. These variables must be given a large uncertainty with time (i.e. lower degree of belief), so that they are allowed to easily change when a new observation is assimilated. Since the distributions of the prior variables are assumed to be Gaussian, we may define a function of time which transforms the Gaussian distribution into a uniform distribution in the time limit. In this way, the distribution of the prior variable begins as a Gaussian distribution, indicating that 95% of the values are within two standard deviations at time t_0 , and with increasing time to the next scheduled observation at time t_1 they become flatter and flatter until the distribution becomes uniform in the time limit for each variable. To account for this temporal constraint, an additional component of variance is

added to the variance of the prior variables to allow for evolution in the time scale.

$$C_{p_{i_{t_1}}} = C_{p_{i_{t_0}}} \left(1 - \left(\frac{t}{\tau_i} \right)^2 \right) + \frac{(p_{imax} - p_{imin})^2}{12} \left(\frac{t}{\tau_i} \right)^2 \quad (4.13)$$

Here i is the variable of interest, p_{imax} and p_{imin} indicate the max and min values of the variable i respectively, t is the number of days between observation at time t_0 and the observation at time t_1 and τ_i is the relaxation time, i.e. the time that it takes for the standard deviation to become equal to the one corresponding to a uniform distribution covering the full possible range of that variable, if the standard deviation would start from zero and then would continue to grow linearly. The variance of the prior variable is unchanged for the same day of observation and it is replaced by the variance of a uniform distribution in the case that the time difference between two observations is equal to the relaxation time. If the time difference between two observations is more than the relaxation time, either the a priori term in the cost function may not be considered anymore or the variance may be replaced with very large values such as the square of the variable variation range.

4.3.4. Measurement covariance matrix

To evaluate the accuracy and precision with which a remote sensing system retrieves land surface properties, a measure of data quality is of importance (Schott, 2007; Wettle et al., 2004). A wavelength-dependent measure would describe system performance and determine the uncertainty in the sensor output radiances (Gao, 1993). The Noise equivalent delta Radiance (NedL) and the Signal to Noise ratio (SNR) are two important measures to describe the quality of radiometric data, providing a quantitative baseline against which different sensors can be compared. The NedL is the change in radiance that produces a signal change equal to the noise level (standard deviation) of the sensor (Schott, 2007). NedL provides a wavelength-dependent measure of inherent system uncertainty, which unambiguously measures the precision in the measured radiance for each spectral band (Dell'Endice et al., 2009). NedL depends on instrumental and environmental SNR of a sensor and can be defined as the reference radiance divided by SNR.

To estimate image noise standard deviation, we have used the bit-plane method proposed by (Aiazzi et al., 2002; Barducci et al., 2005, 2007). The method is preferable to traditional noise estimators, which mostly require selecting an homogeneous area in the image, since it is insensitive to spatial texture of the image. It assumes that noise is stationary (spatially invariant) and has a small or negligible auto-correlation. Bit-planes having an amplitude less than or equal to the noise standard deviation are dominated by noise and they will show a salt and pepper look (Barducci et al., 2007). A bit-plane of a digital image is a data structure made from a set of bits having the same position in the respective binary numbers. A sequence of bit-planes is extracted from the image starting from the less significant bit to explore whether the bit-plane obeys a random distribution. To find noisy bit-planes, for each pixel (in each spectral band) its difference with the four neighboring pixels is computed and the distribution of these differences is analyzed to assess whether the differences are the result of a textured signal or a random noise. These differences are characterized as Bernoulli trials, in which a fully random

bit-plane with equal probable states “1” and “0” would obey a binomial distribution with mean 0.5. If the bit-plane is not noisy, then the mean of the binomial distribution will be between zero and 0.5. A randomness index is defined based on the difference between the expected mean for a noisy bit-plane (0.5) and the estimated mean from the differences.

The noise standard deviation is then computed by an empirically derived equation of such randomness indices (Barducci et al., 2007). We repeat this process over the entire bit-plane sequence and obtain NedL as the noise standard deviation in each spectral band. The diagonal elements of the measurement covariance matrix are filled with the squares of NedL values. The correlation between different spectral bands has been neglected. It is important to notice that, although NedL gives a baseline indication of instrument radiometric performance, the radiometric performance of an instrument arises as a result of many factors and NedL alone should not be considered a complete description of measurement uncertainty (Anderson et al., 2011).

4.3.5. Model parameterization

The constant SLC inputs during the inversion procedure were independently set for each individual crop class in the study area. Table 4.2 summarizes the constant inputs used in the simulations for leaf and canopy. For each crop type, leaf variables such as Cw and Cdm were obtained from the field measurements averaged over crop type. Other leaf and canopy variables and parameters were determined according to expert knowledge and literature (e.g. (Combal et al., 2002; Gonzalez-Sanpedro et al., 2008; Koetz et al., 2005; Verhoef and Bach, 2003b)). Biophysical variables of brown leaves were set to one prototype for all crop types (Table 4.2). The dry soil reflectance spectra (taken from the field measurement data) were assumed to be identical over the study area. The feasible ranges for the free variables are listed in Table 4.3. It has to be noted that fCover is not taken as free variable in this study but instead we set Cv as a free variable to obtain fCover in the inversion, since fCover is an output of SLC and determined by two important variables LAI and Cv (see Eq 4.2)

Table 4.2: Constant input values of the PROSPECT and SLC models for different crop types

Variable(unit)	Leaf				Canopy					
	N(-)	Cw(cm)	Cdm(g/cm ²)	Cs(-)	D(-)	LIDFa(-)	LIDFb(-)	Zeta(-)	Hot(-)	FB(-)
Alfalfa	2	0.017	0.005	0	0	0	-0.15	1	0.05	0
Barley	1.8	0.011	0.005	0	0.3	-0.85	-0.15	1	0.05	0.7
Corn	1.6	0.019	0.005	0.08	0.8	-0.65	-0.15	1	0.05	0.05
Wheat	1.5	0.029	0.007	0.1	1	-0.7	0	1	0.05	0.3
Sunflower	1.5	0.032	0.006	0.05	0	-0.35	-0.15	1	0.05	0.1
Oat	1.6	0.011	0.005	0.5	0.3	-0.35	-0.15	1	0.05	0.25
Onion	2	0.06	0.006	0	0	-0.35	-0.15	1	0.05	0
Fruit	1.7	0.015	0.005	0.1	0.8	-0.7	0	1	0.05	0.15
Vine	1.7	0.017	0.007	0.1	1	0	-0.15	1	0.05	0.3
Garlic	2	0.06	0.01	0	0	-0.7	0	1	0.05	0
Other crops	1.8	0.014	0.005	0	0.8	-0.35	-0.15	1	0.05	0.2
Brown leaf	2	0	0.008	0.7	-	-	-	-	-	-

The MODTRAN4 main parameters used for TOA simulations are given in Table 4.4. The atmospheric visibilities and water vapor columns were obtained from the ground

atmospheric measurements. The rural aerosol model was chosen according to the field campaign report (Brockmann et al., 2011). No atmospheric soundings concurrent with TM image on June 13th were available and we retrieved atmospheric parameters by matching our retrievals of TOC reflectance with the BOA reflectance image data downloaded from USGS website. The atmospheric condition was assumed to be steady over the study area, which is reasonable over areas smaller than few kilometers.

Table 4.3: Statistics of the ground truth measurements for the study area during SEN3EXP 2009, Barrax. The fifth column presents ranges used in the inversion for each variable [min, max], as well as the initial values are given in parentheses

Variable(unit)	Number of Elementary Sampling Units(ESU)	Min	Max	Range [min, max] inversion(initial value)	Relaxation time(day)
LAI (m^2/m^2)	39	0.12	4.9	[0, 6] (2)	30
fCover (-)	39	0.05	0.87	[0, 1] (0.5)	30
Cab ($\mu g/cm^2$)	38	21.4	41.2	[10, 60] (30)	30
LIDFa (-)	-	-	-	[-1, 1] (-0.35)	30
FB (-)	-	-	-	[0, 0.5] (0.1)	30
SM (-)	-	-	-	[0, 0.5] (0.1)	2

4.3.6. Design of retrieval scenarios

Here, we evaluate the influence of prior information on biophysical variable retrieval in a multi-temporal, multi-sensor framework. First, we analyze cases without incorporating prior information from other retrievals into the retrieval problem. This scenario represents the case of single sensor variable retrieval, when only radiometric data are used. In the second case, we begin with the first image (Landsat 13th June) and retrieve the state variables. These retrievals are then used to update relevant properties in the geo-database (see Figure 4.3) and new retrievals are performed using information from the geo-database as prior information. The scenarios have been designed as examples of different temporal sequences and compared with single sensor, single date observations. In addition, we investigated incorporating prior information from identical sensor type against different sensor types in the multi-sensor framework. Four statistical metrics are used for evaluating the performance of the approaches: root mean square error (*RMSE*), coefficient of determination (R^2), bias, and standard deviation (*Std*). For the validation part of this study, since the field ground measurements were collected from 20 to 24th June 2009, we assumed a low variability in time of biophysical variables when evaluating our retrievals with the TM image acquired on June 13th against these ground measurements.

4.4. Results

4.4.1. Forward simulation

The capability of RT models to accurately simulate the spectral radiance of vegetation canopies is a prerequisite of model inversion (Baret and Buis, 2008). Apart from the demonstrated suitability of the *SAIL* family *RT* models in different studies as described in § 4.2.3.1, we have also quantified the agreement between measured satellite radiances and simulated signatures of ground biophysical variables for different crop types

Table 4.4: Input parameters for MODTRAN4 simulations

Parameter	Value
Atmospheric profile	Mid-latitude summer
DISORT	8 streams
CO ₂ mixing ratio	380 ppmv
Aerosol extinction	Rural
Aerosol phase functions	Internal Mie-generated
Stratospheric aerosol	Background profile and extinction
Visibility	23, 40, 25, 45, 40 (km)
Water vapour column	1.7, 1.5, 1.5, 1.4, 1.2 (g/cm^2)
Day of year	164, 170, 171, 172, 173
Sensor altitude	600, 705 km
Target altitude	0.7 km
Target latitude	39°3'N
Target longitude	2°60' W
Interval	1nm
FWHM	5nm
Slit function	Gaussian

in the Barrax study area. The radiance mismatch was evaluated as the RMSE between measured and simulated spectral radiances by the coupled SLC-MODTRAN4 RT model. Figure 4.5 shows, for instance, the comparison of measured CHRIS-Proba and Landsat TM top of atmosphere radiance against the simulations for a corn pixel simulated from field ground measurements. The leaf and canopy properties are set as in Table 4.2 for a corn crop. The simulations generally matched the measured radiances well for both CHRIS-Proba and Landsat TOA radiances in different observation directions. However, a tendency toward overestimation is seen in the visible with a relatively large discrepancy (the middle red circle in Figure 4.5 top left) persisted around the green spectral region for all forward simulations in the CHRIS-Proba dataset corresponding to the chlorophyll sensitive region. Since this discrepancy was found in all the simulations, it is probably due to sensor calibration or uncertainty in ground measurements of chlorophyll content. Therefore, the spectral bands (5 spectral bands) located in this region were excluded from our analysis. Besides, the first spectral band and band 39 (oxygen sensitive band) of the CHRIS-Proba sensor are highly corrupted by noise and they were also neglected in the inversion procedure.

4.4.2. Sensitivity analysis and dimensionality

To assess the actual influence of a given factor on the modeled radiance, the total-order sensitivity effect of the factor is considered, which includes both the main effect and the interaction effects with other factors. We can only retrieve influential factors and the other factors are fixed to the values stored in the database. Figure 4.6 shows the sensitivity of TOA radiance to surface properties for the Landsat TM image and the CHRIS-Proba image. The results for the ASTER image have not been shown for the sake of brevity and

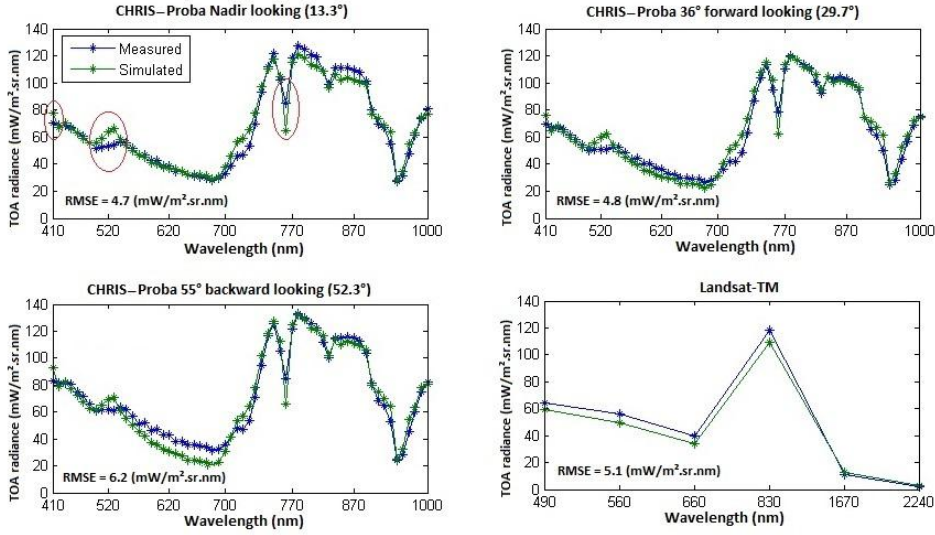


Figure 4.5: Comparison between actual CHRIS-Proba (19th June) and Landsat TM (22nd June) (bottom right) top of atmosphere radiance against the simulations for a corn pixel with ground truth measured LAI ($2.9 \text{ m}^2/\text{m}^2$), fCover (0.6), Cab ($38 \text{ } \mu\text{g}/\text{cm}^2$), Cdm ($0.005 \text{ g}/\text{cm}^2$), Cw (0.019 cm) and LIDF (LIDFa: -0.65 and LIDFb: -0.15) with the sun zenith angle 30° and 25° for CHRIS-Proba and Landsat TM respectively. The red circles (top left) representing noisy bands (i.e. the first band (left) and band 39 (right)) or bands with a large discrepancy (middle) were neglected in the analysis

since there were only three spectral bands in the visible having very similar pattern with the corresponding Landsat visible bands. The sensitivities to 19 inputs (out of 23 SLC inputs) are shown in Figure 4.6. Soil moisture is the only soil related variable considered in the study and the other soil factors were not applicable due to employing a dry soil reflectance spectra taken from field measurements.

In the case of CHRIS-Proba image (Figure 4.6 top), crown coverage (C_v), leaf area index (LAI), leaf inclination distribution function ($LIDFa$), soil moisture (SM), chlorophyll content of green leaves ($Cabg$) and fraction of brown leaves (FB) were identified as the most influential variables determining the TOA radiance over most of all the CHRIS-Proba spectral bands. The intrinsic dimension of the full set of multi-angular CHRIS-Proba images was estimated to be 7. Since this is an upper bound on the true intrinsic dimensionality, the six mentioned variables were set as free variables in the inversion. For the Landsat images, the state variables C_v , LAI , $LIDFa$, SM and $Cabg$ were identified to be the most influential variables based on the results of the sensitivity analysis (Figure 4.6 bottom). Though, since the intrinsic dimension of the Landsat TM images was found to be 5, we retrieved only four variables C_v , LAI , SM and $Cabg$. In the case of ASTER, similar to Landsat, C_v , LAI , SM and $Cabg$ were influential. However, the dimension of the ASTER dataset was three and to be consistent with other datasets we kept soil moisture fixed with values extracted from the database and C_v , LAI and $Cabg$ were free variables.



4.4.3. Variable retrieval results

4.4.3.1. Single sensor variable retrieval results

It is apparent from Table 4.5 that in the case of single sensor variable retrieval best

Table 4.5: The accuracy of the estimation of three vegetation state variables in the case of single sensor variable estimation. The metrics used are: the root mean square error (*RMSE*), the coefficient of determination (R^2), the bias (Bias) and the standard deviation (*Std*). A positive (negative) bias indicates an overestimation (underestimation) of the estimations

	LAI				fCover				Chlorophyll content			
	RMSE(m^2/m^2)	R^2	Bias	Std	RMSE(-)	R^2	Bias	Std	RMSE($\mu g/cm^2$)	R^2	Bias	Std
Landsat-TM (13 th June)	1.27	0.15	0.30	1.24	0.20	0.47	-0.10	0.17	11.62	0.01	7.83	8.58
CHRIS-Proba (19 th June)	0.80	0.62	0.32	0.74	0.12	0.78	-0.07	0.11	10.68	0.24	8.12	6.93
CHRIS-Proba (20 th June)	0.86	0.56	0.36	0.78	0.14	0.71	-0.04	0.13	11.90	0.07	9.09	7.67
ASTER (21 st June)	1.14	0.43	0.83	0.78	0.15	0.56	-0.07	0.14	10.42	0.03	-6.34	10.42
Landsat-TM (22 nd June)	1.09	0.48	0.66	0.87	0.15	0.63	-0.06	0.14	11.71	0.01	-4.64	11.41

accuracy was achieved using CHRIS-Proba for all variables. This could be explained, because CHRIS-Proba provides hyperspectral multi-angular imagery with relevant spectral bands for a significant angular and spectral sampling of canopy BRF. This allows to study anisotropic vegetated areas and to retrieve relevant vegetation characteristics such as LAI and fCover. Having more spectral and angular bands increases the dimensionality of the dataset making LIDFa and FB retrievable as well. This leads to a better characterization of canopy architecture and to a better modelling of non-photosynthesis vegetation parts. LAI, fCover and Cab were retrieved with RMSE of 0.80 (m^2/m^2), 0.12 and 10.68 ($\mu g/cm^2$) respectively from the CHRIS-Proba dataset on 19th June and with RMSE of 0.86 (m^2/m^2), 0.14 and 11.90 ($\mu g/cm^2$) from the CHRIS-Proba dataset on 20th June. The independent retrievals from the two CHRIS-Proba images were comparable, although the results were slightly better for the dataset on 19th June because of better angular sampling since all the five angles were used for the dataset on 19th June versus the three angles used in the dataset on 20th June; also the nadir image on 20th June was not covering the entire study area.

Overall, retrievals from the Landsat image on 13th June show a lower accuracy than the other images with RMSE 1.27 (m^2/m^2), 0.20 and 11.62 ($\mu g/cm^2$) for LAI, fCover and Cab respectively. Such results are partly explained by the time gap between the ground measurements and the acquisition time of the image. For instance, NDVI values (not shown) and visual inspection (see Figure 4.8) of the alfalfa fields from 13th to 22nd June show significant variation which is likely due to alfalfa regular cut before the acquisition of the first image. This implies that the assumption of invariant vegetation properties over a short period of time used in some studies (Lauvernet et al., 2008) does not hold for some crop types such as alfalfa with regular cut and fast growing stands. Retrievals from the ASTER image on 21th June also showed rather low accuracy with RMSE of 1.14 (m^2/m^2), 0.15 and 10.42 ($\mu g/cm^2$) for LAI, fCover and Cab respectively, because only three spectral bands were used for the retrieval. The bias values in Table 4.5 show overall overestimation for LAI and underestimation for fCover.

4.4.3.2. Multi-sensor variable retrieval results

Table 4.6 compares the results obtained with the multi-sensor variable retrieval in terms of four statistical metrics per image. More detailed comparisons are given in Figure 4.7

for each crop type. Comparing the results of Table 4.5 (single sensor) and Table 4.6 (multi-sensor), an improvement is seen in the case of multi-sensor versus single sensor for all scenarios. In general, the RMSE, bias and standard deviations of the multi-sensor approach are smaller than those of the single sensor approach. The improvement was more significant when prior information came from hyperspectral sensor (CHRIS-Proba). The RMSE value of LAI retrieval has decreased from $1.09 (m^2/m^2)$ to $0.70 (m^2/m^2)$ and from $1.14 (m^2/m^2)$ to $0.72 (m^2/m^2)$ applying multi-sensor retrieval for Landsat and ASTER, respectively. Similar improvements were found for fCover: RMSE values decreasing from 0.15 in both cases to 0.10 and 0.11 for Landsat and ASTER images, respectively. The better performance of incorporating prior information from the CHRIS-Proba over the other sensors can be explained by two main factors. First, having a higher number of free variables permits updating and improving the values for more variables in the geo-database and thus more realistic values of the state vegetation variables. Second, better retrievals from more spectral bands would produce smaller variance values of the retrievals and consequently increases the weights given to the prior term in the cost function. This forces the cost function to achieve a balance between the prior term and the radiometric term and hence it does not allow the solution to be very far from the prior solution unless the radiometric term is considerable which indicates actual change in that variable.

There is a significant positive R^2 between retrievals of LAI and in particular fCover (with more than 0.80 for all cases) versus ground measurements in the multi-sensor approach. This is in part due to the capability of the SLC in modeling gap fraction in vegetation canopies. The SLC measures effective fCover from the extinction coefficient in vertical direction which is linked to leaf angle distribution, vertically projected crown cover fraction (Cv) and LAI for canopy. Having LAI, Cv and LIDFa as free variables helps to better model fCover using SLC than its predecessor version of SAIL radiative transfer model. Another reason for this is due to the potential of multi-angular data to better explore the canopy structure in the case of CHRIS-Proba, as it has been already reported (Barnsley et al., 2004). In consideration of the bias values in Table 4.6, an overestimation of about $0.30 (m^2/m^2)$ is seen for all LAI retrievals, while fCover retrievals are underestimated with an average of 5%. LAI overestimation by SLC has been already reported in Laurent et al. (2013).

Table 4.6: The accuracy of the estimation of three vegetation state variables in the case of multi-temporal, multi-sensor variable estimation

	LAI				fCover				Chlorophyll content			
	RMSE(m^2/m^2)	R^2	Bias	Std	RMSE(-)	R^2	Bias	Std	RMSE($\mu g/cm^2$)	R^2	Bias	Std
Landsat-TM (13 th June)	-	-	-	-	-	-	-	-	-	-	-	-
CHRIS-Proba (19 th June)	0.75	0.68	0.34	0.66	0.12	0.82	-0.05	0.11	9.99	0.34	7.72	6.33
CHRIS-Proba (20 th June)	0.69	0.74	0.34	0.60	0.11	0.85	-0.05	0.10	10.79	0.38	8.93	6.05
ASTER (21 st June)	0.72	0.73	0.36	0.63	0.11	0.83	-0.05	0.10	9.40	0.29	6.87	6.41
Landsat-TM (22 nd June)	0.70	0.71	0.29	0.64	0.10	0.85	-0.04	0.10	8.69	0.17	2.92	8.19

Despite the considerable improvements in LAI and fCover values, chlorophyll con-

tent retrievals are not generally in good agreement with ground measured data neither for the single sensor variable retrieval nor in the multi-sensor approach. In the best case scenario, the RMSE value of $8.69 \text{ } (\mu\text{g}/\text{cm}^2)$ with the R^2 of 0.17 was obtained for the Landsat image on 22nd June in the multi-sensor approach. Overall, the results of Cab has improved slightly applying multi-sensor approach, however, resulting R^2 and bias values do not provide evidence supporting strong relationship between retrievals and ground measurements.

Results from the multi-sensor variable retrieval are also plotted in terms of crop type for different sensors in Figure 4.7. The top row shows the LAI retrievals versus ground measurements, the middle row represents the comparisons of fCover and the bottom row shows the results of Cab retrievals against ground truth data.

It is seen from Figure 4.7 that crop classes with LAI values lower than one (such as fruit, vineyard and onion) were mostly overestimated in all cases. This might be explained by a number of different factors. The background soil reflectance contributes significantly to the output radiance at low vegetation densities as with LAI values less than one. Consequently, the assumption of invariant soil type might lead to some inaccuracy in the retrievals. In this sense, the model tries to find the best match between observed and modeled radiances by varying LAI values in order to compensate for the changes in soil reflectance. Also, this might be partly due to the turbid medium nature of the canopy RT model. The canopy is described by the 4SAIL2 as a two-layer turbid medium with clumping effect only for crowns. The turbid medium approach, by definition, assumes the canopy to be a homogenous medium of infinitesimal scatterers. Therefore, less homogenous vegetation cover and the absence of clumping for all levels (e.g. stem, shoot and branch) might explain the slight tendency to overestimation of LAI. Accordingly, when the situation is close to the turbid medium assumption, the model delivers better agreement with ground measured data as with higher LAI values.

In terms of crop type, the retrievals of LAI and fCover for garlic, corn and sunflower crops were very close to the measured values in particular for fCover values. Again, these results are likely because of better model characterization and situation of such crops closer to the model assumption (e.g. the turbid medium assumption used in 4SAIL2). However, LAI and fCover for alfalfa were underestimated for all cases regardless of implementing single sensor retrieval or multi-sensor approach. It is difficult to explain this result, but it might be related to either inaccuracy in ground measurements or some unknown factors such as flowering which is not taken into account in RT models. Visual inspection of the photographs taken from the fields and as well as the comparison of the spectral response of alfalfa pixels to other samples taken from other field campaigns do not correspond to very high LAI values as recorded during the field measurements. As discussed before, the performance of the two approaches was poor in retrieving chlorophyll content values. The chlorophyll content was overestimated for almost all crop types. The reason for this is not clear.

Figure 4.8 illustrates the results of incorporating identical sensors versus various sensor types information on the performance of variable retrieval of the Landsat image on 22nd June. Referring to Figure 4.8, it can be inferred that best performances are generally obtained by the multi-sensor approach combining information from different sensor types. Incorporating information from identical sensors (the middle column in Fig-

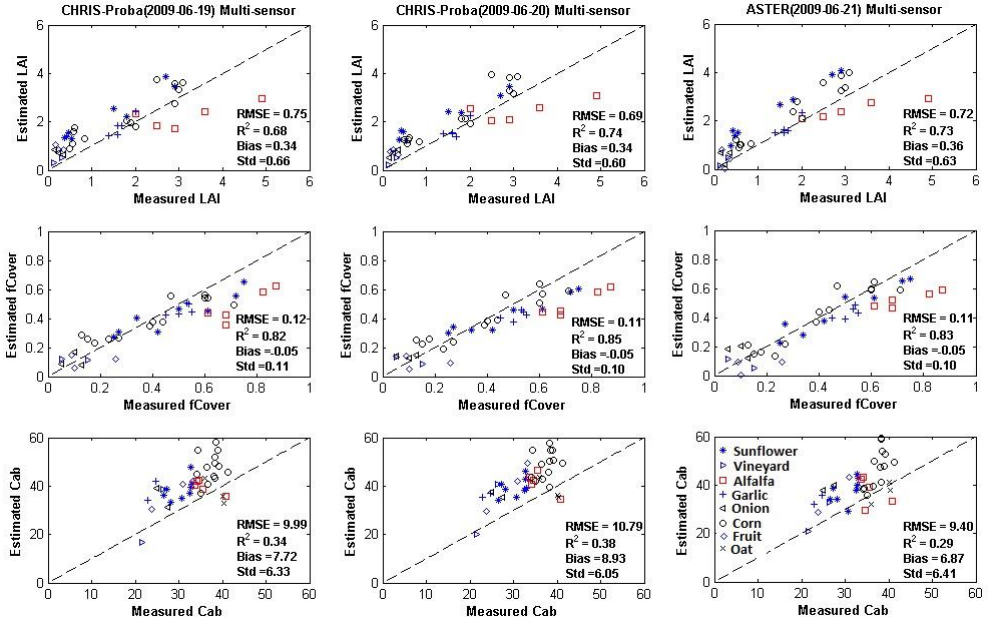


Figure 4.7: Multi-sensor variable retrieval for LAI, fCover and Cab using CHRIS-Proba and ASTER images. Estimated values from CHRIS-Proba on 19th June (left column), estimated values from CHRIS-Proba on 20th June (middle column) and estimated values from ASTER on 21st June (right column). The results of the Landsat image on 22nd are shown in Figure 4.8

ure 4.8) has improved the results slightly decreasing the RMSE values from 1.09 to 1.00 (m^2/m^2) for LAI, from 0.15 to 0.14 for fCover and from 11.71 to 10.03 ($\mu g/cm^2$) for Cab. However, the best performance was achieved using information from different sensor types characterized with a decrease of the RMSE from 1.09 to 0.70 (m^2/m^2) for LAI, from 0.15 to 0.10 for fCover and from 11.71 to 8.69 ($\mu g/cm^2$) for Cab. Similarly, the bias has decreased from 0.66 to 0.29 (m^2/m^2) for LAI, from 6% to 4%. for fCover. This, in fact, is not surprising, because the differences in the spectral and angular sampling, spectral sensitivity and temporal resolutions of different sensors potentially offer a source of complementary information for variable retrieval where it would yield better retrievals of biophysical variables. Furthermore, the results support the hypothesis that a set of data types with diverse sensitivities to vegetation variables would lead to more accurate results than those for any single data type.

The traditional optimization algorithms are computationally intensive, and solution time linearly depends on the problem dimensionality. The dimensionality of a problem, in turn, is a factor of the number of free variables to be retrieved and the number of spectral and angular bands involved in the inversion. In the case of single sensor variable retrieval, the average number of iterations was 19, 23, 20, 10 and 17 for Landsat (13th June), CHRIS-Proba (19th June), CHRIS-Proba (20th June), ASTER (21st June) and Landsat (22nd June) respectively. The average number of iterations decreased while applying the multi-sensor approach and it was 7, 5, 4, and 4 iterations for CHRIS-Proba

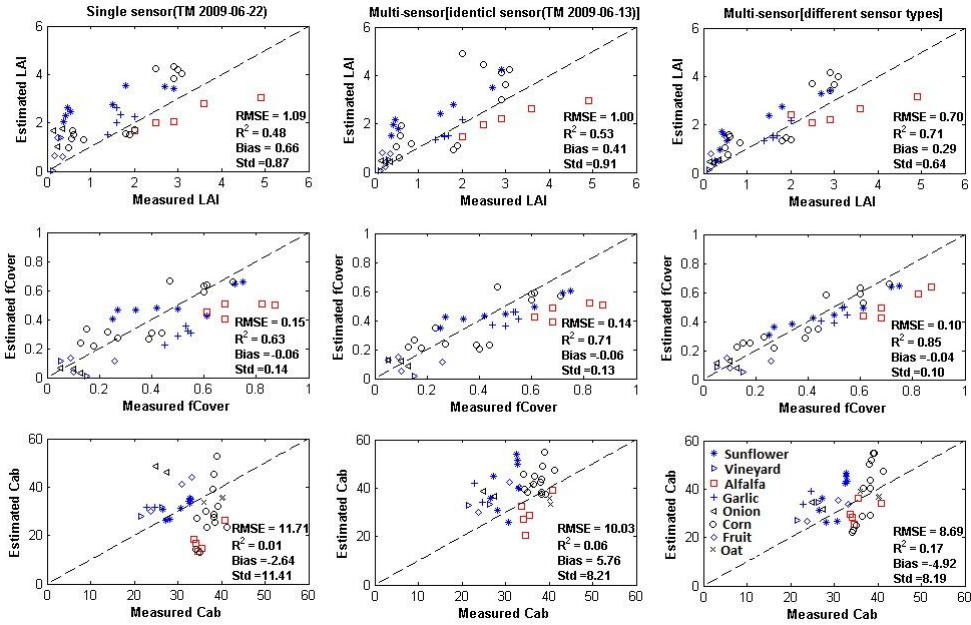


Figure 4.8: Multi-sensor variable retrieval for LAI, fCover and Cab in terms of sensor type. Single sensor retrievals (left column), multi-sensor retrievals using prior information from identical Landsat image on 13th June (middle column) and multi-sensor retrievals combining information from different sensor types (right column)

(19th June), CHRIS-Proba (20th June), ASTER (21st June) and Landsat (22nd June), respectively.

4.4.3.3. Difference map of biophysical variables

The retrievals of LAI and fCover from the Landsat image on 22nd June (last acquired image) were subtracted from the values derived by the Landsat image on 13th June (first acquired image). The resulting difference maps are shown in Figure 4.9. This analysis is concerned with fields where the two retrievals give noticeably different LAI and fCover values. Regions where the LAI and fCover is lower on 13th June than 22nd June are those with positive values and regions with negative values indicate higher LAI and fCover on 13th June. The time series of LAI and fCover averaged over the labeled fields are also shown in this figure. Figure 4.9 shows that significant negative deviations in both LAI and fCover values occur for some fields such as the rape field (labeled “A”), the rye grass field (labeled “B”) and the garlic field (labeled “C”). It can be seen from the RGB images (Figure 4.9 left) that these fields had dense vegetation cover in the first image where the fields show very low vegetation cover in the image on 22nd June. In contrast, for some fields such as the sunflower field (labeled “D”) and the alfalfa field (labeled “E”) vegetation cover was low in the first image while vegetation covers seem better developed in the last image. The alfalfa field was cut before the acquisition of the first image and since

alfalfa grows fast we see an obvious increase for LAI and fCover values in the last image for the alfalfa field. The sunflower field was also at early growth stage in the first image and has developed at the time of the last image. However, apart from temporal changes due to crop phenology, for some fields the variation is rather related to the retrieval accuracy. For instance, LAI was overestimated for the garlic field (labeled "F") in the first image. Overall, large parts of the maps are characterized with small positive or negative deviations for different crop types indicating small changes which in most cases are related to better retrievals of variables from the multi-sensor approach for the image on 22nd June.

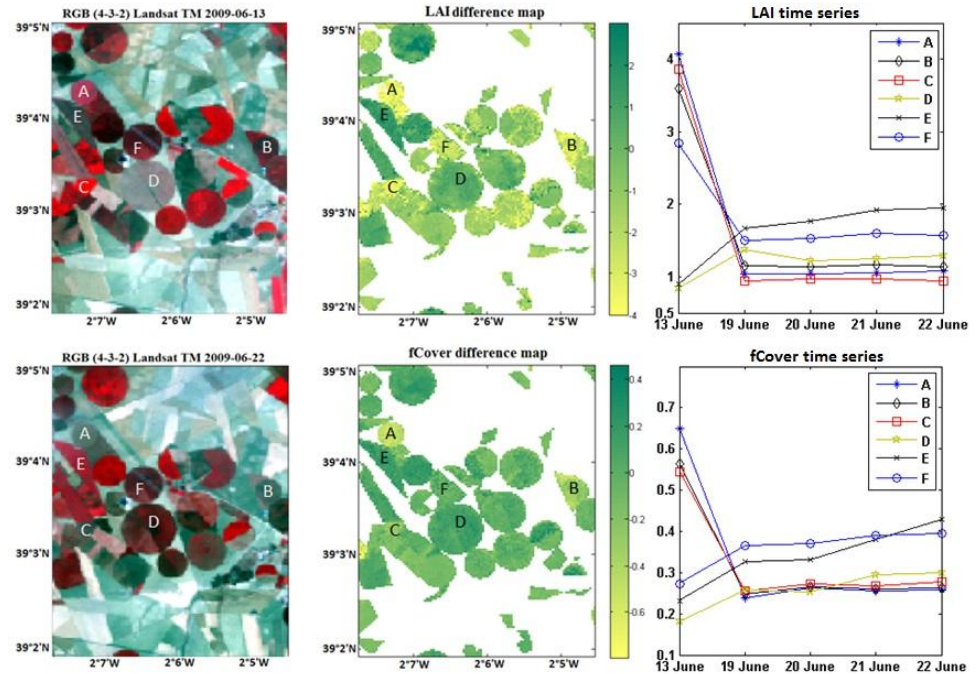


Figure 4.9: RGB (4–3–2) band combination for the Landsat image 13th June (top left) and for the Landsat image on 22nd June (bottom left). Difference maps between LAI (top middle) and fCover (bottom middle) values estimated from the Landsat image on 22nd June and the Landsat image on 13th June. The letters represent different fields: "A" (Rape), "B" (Rye Grass), "C" (Garlic), "D" (Sunflower), "E" (Alfalfa), "F" (Garlic). The time series of LAI (top right) and fCover (bottom right) are averaged over the labeled fields. The Landsat images are TOA radiance images and hence the atmospheric impact has to be taken into account for the interpretation of the images. This influence is specifically significant on visible and the infrared radiation, where atmospheric scattering causes gain on the radiation reaching the sensor

4.4.3.4. Maps of retrieved biophysical variables

Maps of the six retrieved biophysical variables for Barrax site are plotted in Figure 4.10. The maps are the final products of the multi-temporal, multi-sensor approach after the last acquired image (i.e. Landsat 22nd June) as stored in the geo-database. The figure provides an evaluation of how the approach functions over the vegetated fields in the

study area. It can be seen that LAI varied from 0 to 5.5 over the study area, with fields, such as corn and sunflower, at their early growth stage having values of less than 2 and fields with closed canopy cover, such as oat and wheat, had LAI values of the order of 3 to 5.5. The figure shows a range in fCover between 0 and approximately 0.9. The highest values of fCover occurred in the wheat, barley and oat fields with values exceeding 0.7. Comparing the results of LAI and fCover, it is evident that there is a significant relationship between the two factors in which the fields with high LAI also had high vegetation cover indicating well-developed canopies. No LAI and fCover ground measurements were available for wheat and barley and it is seen that these fields had very high LAI and fCover. These results are in accordance with the field campaign report (Brockmann et al., 2011) and complementary information (e.g. photographs) provided during the campaign. Figure 4.10 shows that there are within field variations of different variables for some fields with different crop types. These within field variations are likely due to local soil condition variability or because of farm management practices.

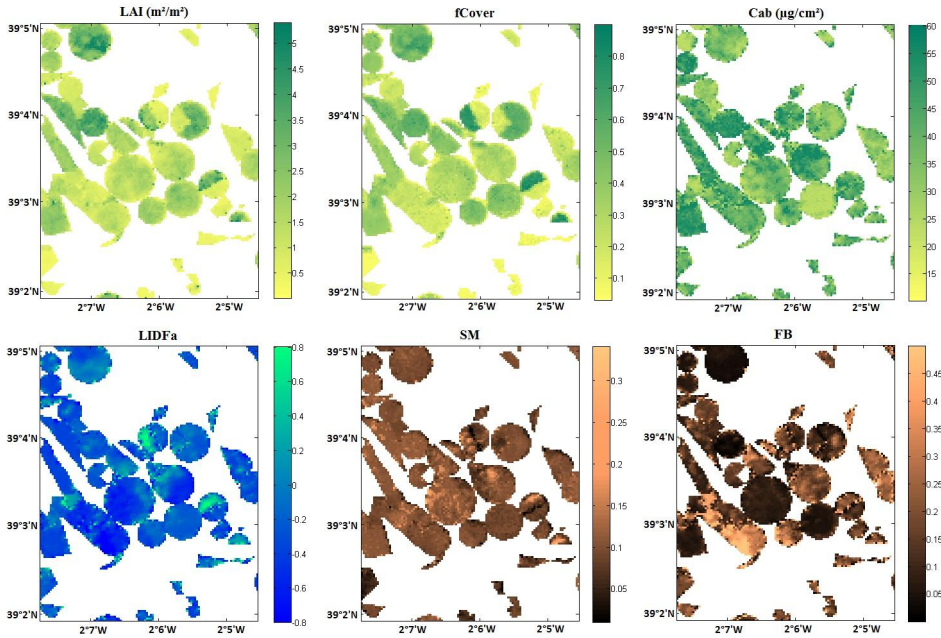


Figure 4.10: Maps of the retrieved biophysical variables over the Barrax area for LAI, fCover, LIDFa, SM, Cab and FB. These maps are the final products of the multi-temporal, multi-sensor approach after the last acquired image (i.e. Landsat 22nd June) as stored in the geo-database

The values of the LIDF parameter “a” varied from −0.8 to 0.8 indicating a variety of leaf angle distribution types from erectophile to planophile, even though the majority of fields are still presenting spherical like leaf angle distribution. On the one hand, the leaf angle distribution map shows rather unique pattern per field which is consistent with those of other studies proposing to assume this parameter constant per field (Atzberger and Richter, 2012). On the other hand, in some cases within field LIDF-variations are still

considerable suggesting that LIDF contributes to a more accurate simulation of canopy angular and spectral signature. Spatial variations in LIDF are observed in fields with multiple crops (see Figure 4.1) or fields with the same crop but at different phenological stages, clearly visible in the TM images (Figure 4.9). Leaf chlorophyll content values varied between 10 and 60 ($\mu\text{g}/\text{cm}^2$), and as discussed before, were overestimated in most fields which is in contrast with ground measurements. The values of the fraction of brown (FB) leaves varied from 0 to 0.5 having the highest values for wheat and barley fields which were senescent at the time of the field campaign (see Figure 4.1 for field cover type). Indeed, this is an interesting feature of the SLC that accounts for the brown leaves and makes it more flexible to model leaf senescence. There were no ground FB measurements, but the results match the information given in the campaign report. Soil moisture content, as shown in Figure 4.10, was retrieved to be less than 40% for all fields where high soil moisture content refers to irrigated fields and low soil moisture content correspond to dry fields. Unfortunately, we had no ground measurements of soil moisture content to evaluate the retrievals. However, the soil moisture variation obtained in this way is rather a substitute for the soil brightness variations than the actual soil moisture content.

The maps shown in Figure 4.10 are the mean values of the posterior distribution for each variable. The Bayesian inversion also provides an uncertainty estimate for the retrievals. This uncertainty can be viewed as a measure of the reliability and quality of the retrievals. The uncertainty maps (i.e. standard deviation) of Cab, fCover and LAI are shown in Figure 4.11. The interpretation of these maps should be relative to the retrieved values. A higher absolute uncertainty does not necessarily mean that the variable is retrieved poorly or similarly a very low value does not guarantee reliable retrieval. Therefore, a relative uncertainty measure would provide a better interpretation of the uncertainty of the retrievals (Verrelst et al., 2013b). The relative uncertainty can be calculated as the standard deviation of the retrievals divided by their retrieved value. The relative uncertainty of the irrigated circular fields with high LAI values was mostly between 2% to 20% and increased for fields presenting very low LAI values. A similar behavior was observed for fCover and Cab uncertainty maps over the irrigated circular fields. However, fields with very low fCover showed higher relative uncertainty than in the case of LAI.

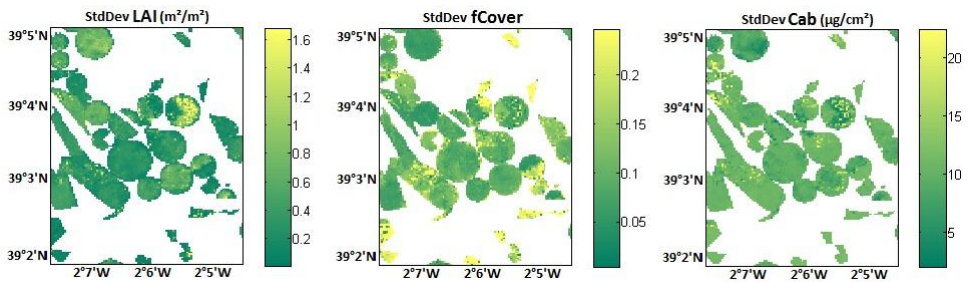


Figure 4.11: Maps of the uncertainty (i.e. standard deviation) of the retrieved biophysical variables of the multi-temporal, multi-sensor approach after the last acquired image (i.e. Landsat 22nd June) over the Barrax area for LAI, fCover and Cab

4.5. Discussions

4.5.1. TOA radiance simulation

As discussed in § 4.4.1, the simulations done with ground measurements as input were generally in good agreement with the measured radiance data. However, in some cases the RMSE values between the simulated and measured radiances tend to increase, for example when increasing the viewing angle. Additionally to the reasons given in § 4.4.1, some assumptions on which the simulation are based might introduce some uncertainty. For instance, the adjacency effect has not been considered in the simulations and it might cause some inaccuracies. The reason for neglecting is that the inversion is pixel-wise and cannot use the average bi-hemispherical reflectance over surroundings of the pixel. However, this problem is mitigated when the surroundings are homogeneous such as agricultural areas with same crop type and large scale fields.

4.5.2. Computational considerations

Traditional optimization algorithms suffer from large computational burden due to the large numbers of iterations usually required to minimize a given cost function. The sequential Bayesian algorithm can reduce this computational time considerably. In fact, if one can assume that previous observations have led to surface properties that are already well “on track”, then we just need to move a little bit from the previous solution to find the new solution and the method converges very fast. Our study further demonstrated that the number of iterations decreases with the Bayesian multi-sensor approach compared to the cases of independent retrieval. This is crucial in the implementation of such algorithms while working with large satellite datasets. However, the approach would be very computationally demanding for application on a per pixel basis for global studies compared to lookup tables and machine learning algorithms. On the other hand, lookup tables and machine learning algorithms, despite their common use in variable retrieval due to ease of use and computational efficiency, become less practical in the case of multi-sensor approach and present serious challenges because of the high dimensionality of datasets and variable conditions from one sensor to another (e.g. observation conditions, number of inputs/outputs etc.). To conclude, for operational mapping of vegetation state variables, the computational time of the presented approach is still a crucial consideration and has to be reduced before extending the approach for regional and global applications.

4.5.3. Observation and a priori covariance matrices

The heart of the Bayesian approaches is the a priori knowledge expressed by the prior term in the cost function. The degree of belief in the a priori knowledge is determined by the (co)variance matrix of a priori knowledge. This (co)variance matrix may be estimated empirically using expert knowledge and ancillary ground measurements (Combal et al., 2002). Due to the lack of ground measurements and also the limitations of such an estimation in which a value should be assigned to a crop class (or field), we found this approach less practical in the multi-temporal, multi-sensor approach. Another way of estimating this covariance matrix is to use the spatial heterogeneity over each crop field. In such a way the fields are assumed to be homogenous and the variation of the retrievals

of an observation over a field is taken as the covariance matrix of the a priori information for the successor observation. Having done some preliminary analysis (not shown), we have noticed that this approach can be beneficial when within-field variations are negligible. However, when within-field variations are significant or the retrievals are precise but not accurate (i.e. very small variance), this approach may lead to wrong judgment on the accuracy of the a priori information. Therefore, we have used the covariance matrix of the retrievals which includes the uncertainty of the radiometric part plus the uncertainty of the previous prior information (see Eq 4.11). The posterior covariance is estimated by the inverse of the Hessian matrix at the optimal solution. This appears to be a reasonable way to express the degree of our belief in the prior retrievals. Overall, the cost of the prior term in the cost function is usually small compared to the cost of the radiometric term. It might seem that the effect of the prior term is not influential on the main cost function and the decision is made more based on the radiometric cost. Contrariwise, incorporating prior information is very important to avoid the inversion becoming ill-posed and since the solution should be around the prior value, even small cost of the prior information plays a crucial role in the retrieval problem.

The observation covariance matrix must include uncertainties in both observation and forward model (Kimes, 2000). It is not feasible to assess forward model uncertainties without a source of perfect reference observations, and therefore they are usually neglected (Widlowski et al., 2007). Consequently, for the observation (co)variance matrix, we have used the variance matrix filled by the squares of the wavelength-dependent NedL values assessed from observations. This seems to be an appropriate form of weighting different spectral bands based on a measure of data quality, although it still does not take the correlation of spectral bands into account and moreover NedL alone may not provide a full characterization of the sensor quality.

4.5.4. Sensitivity analysis

Global sensitivity analysis provides complementary information to the variable retrieval by identifying the most influential variables given the measurements. It is not always an easy task to choose a variable that is influential or non-influential over the entire range of the spectrum. One way to tackle this challenge is to design inversion techniques that retrieve one variable at a time using the most sensitive spectral bands to the variable of question while insensitive to others. However, in practice, with the available inversion techniques, we have to determine free variables prior to the inversion. In this sense, it is a common assumption to find the most influential variables in terms of their average sensitivity values over the entire spectral bands. Therefore, we have selected retrievable variables based on their average influence over the spectral bands of the given sensor.

4.5.5. Additional error sources

There are a number of issues that might affect the accuracy of the retrievals in this study by introducing errors at various stages of the inversion and need further investigation. An issue is related to the scaling effect of the ground measurements to which the retrievals are compared. This scaling problem is both for spatial scaling and temporal scaling. The former refers to the fact that ground measurements are carried out on small sampling points with a few meters to measure vegetation properties (e.g. as in Barrax)

while the pixel size of satellite images are often larger than a few tens of meters (e.g. CHRIS-Proba with 34m pixel size). Additionally, the sampled points were restricted to a limited number of fields and not covering all conceivable situations. The temporal scaling also indicates the time difference between the ground measurements and satellite data. This might be considered as negligible for a few days depending on vegetation type. However, in the case of crops, this effect is relevant for some specific crops as they grow very fast. For instance, the alfalfa fields in the study area presented very little vegetation cover for the image on 13th June while they showed dense vegetation cover in the image on 22nd June. We have used a penalty function (i.e. Eq 4.13) for temporal scaling to cope with this problem, though, the values used for relaxation time are extracted empirically and might change based on vegetation type.

Another issue is the assumption of invariant soil type and the use of a local soil reflectance spectra over the study area. For the soil reflectance spectra, if no prior information of the soil type and soil optical properties is available, it is a common practice to use soil pixels in the image and extract a mean dry soil reflectance spectra, for example (Dorigo et al., 2009; Laurent et al., 2014) to insert as input for SLC. The modified Hapke's model implemented in SLC is able to capture the spectral effects of soil moisture variations all over the solar reflective spectral domain. However, this assumption might lead to some inaccuracy in the results in particular for low vegetation cover as earlier discussed in section 4.3.2. Finally, the focus of this study was the retrieval of LAI, fCover and chlorophyll content and the other retrieved variables such as LIDF and FB were qualitatively interpreted. However, it would be important for future studies to evaluate the retrieval of the other variables in the same quantitative manner as done here for LAI, fCover and Cab.

4.6. Conclusions

In this study, we present a prototype proof of concept of a multi-temporal, multi-sensor approach to retrieve vegetation properties using spectral-directional radiometric data. The procedure described and evaluated in this study is designed for the exploitation of a temporal sequence constructed by combining data acquired by different sensors over time. We focused on the retrieval of LAI, fCover and leaf chlorophyll content from top of atmosphere radiance data over the Barrax agricultural test site for a range of crops. A Bayesian optimization approach was used to invert the coupled SLC-MODTRAN4 RT model to retrieve vegetation properties from a temporal sequence of different satellite observations including, in this case study, CHRIS-Proba, Landsat TM and ASTER. The bit-plane method was applied to estimate observation (co)variance matrix, and the posterior covariance matrix of retrievals from one observation was used as prior (co)variance matrix for the successor retrieval procedure.

The results of this study document the importance of incorporating prior information into the retrieval of biophysical variables. In our study, this information comes from the retrievals of the previous observation (image data). The method stores the surface properties in a geo-database and target properties are updated by means of satellite observations. When a new observation is acquired, a sensitivity analysis is used to identify the retrievable variables with respect to the dimensionality of data and these variables are updated in the geo-database. The study demonstrates that integrating information

from different satellite observations improves the retrievals of LAI and fCover. Although the approach retrieved structural variables with reasonable accuracies, the agreement between retrieved and measured values for leaf chlorophyll content was poorer. A possible explanation of this may be the lack of enough chlorophyll sensitive spectral bands in the inversion since some of the sensitive bands were excluded because of the problem addressed in § 4.4.1. The overestimation of chlorophyll content might also be related to some inaccuracy either in the RT model parameterization or ground measurements due to the limited range in chlorophyll content sampled by ground measurements. Marginal improvement was also observed for cases where either the time gap between the two images was significant or when two identical sensors are combined within a short time period compared with combining different sensors.

The study also shows the usefulness of the Bayesian model inversion in biophysical variable retrieval. Different aspects of Bayesian model inversion are discussed. This study proposes a new approach for multi-temporal, multi-sensor variable retrieval combining the strengths of Bayesian inference and data from a variety of different sensors. We believe this is an effective way to combine multi-spectral data acquired by different sensors over time, thus increasing the frequency of usable data and of maps of retrieved vegetation properties. This could be, for instance, applied to different sequences of sensors and data, either current (e.g. Landsat, SPOT, Rapid Eye etc.) or future (e.g. Sentinel 2 and 3). The outcomes of the study are an important contribution to further improving the variable retrieval using data from different observations. The approach allows reducing uncertainties of retrievals of vegetation state variables and thus increasing the quality of retrieved vegetation products.

Two issues are identified that warrant further research. First, the computational time has reduced largely using the multi-temporal, multi-sensor approach, compared to the single sensor retrievals. However, the computational time is still a crucial consideration for operational mapping of vegetation biophysical variables for regional and global applications and has to be decreased considerably. Further research will need to focus on computational complexity issues. The second issue concerns a better validation both in terms of time variability and also including more satellite observations, in particular future missions such as Sentinel 2 and 3.

5

Modeling Top of Atmosphere radiance over heterogeneous non-Lambertian rugged terrain

Abstract: Topography affects the fraction of direct and diffuse radiation received on a pixel and changes the sun-target-sensor geometry, resulting in variations in the observed radiance. Retrieval of surface-atmosphere properties from top of atmosphere radiance may need to account for topographic effects. This study investigates how such effects can be taken into account for top of atmosphere radiance modeling.

In this paper, a modeling system for top of atmosphere radiance modeling over heterogeneous non-Lambertian rugged terrain through radiative transfer modeling is presented. The paper proposes an extension of “the four-stream radiative transfer theory” (Verhoef and Bach 2003, 2007 and 2012) mainly aimed at representing topography-induced contributions to the top of atmosphere radiance modeling. A detailed account for BRDF effects, adjacency effects and topography effects on the radiance modeling is given, in which sky-view factor and non-Lambertian reflected radiance from adjacent slopes are modeled precisely. The paper also provides a new formulation to derive the atmospheric coefficients from MODTRAN with only two model runs, to make it more computationally efficient and also avoiding the use of zero surface albedo as used in the four-stream radiative transfer theory.

The modeling begins with four surface reflectance factors calculated by the Soil-Leaf-Canopy radiative transfer model SLC at the top of canopy and propagates them through the effects of the atmosphere which is explained by six atmospheric coefficients, derived from MODTRAN radiative transfer code. The top of the atmosphere radiance is then convolved with the sensor characteristics to generate sensor-like radiance.

Chapter 5 is based on:

Mousivand, A., Verhoef, W., Menenti, M. & Gorte, B. (2015). Modeling Top of Atmosphere radiance over heterogeneous non-Lambertian rugged terrain. *Remote Sensing*, 7(6), 8019-8044.

5.1. Introduction

Top-Of-Atmosphere (TOA) radiometric data are traditionally converted to Top-Of-Canopy (TOC) reflectance before being used for variable retrieval (Laurent et al., 2011a). This conversion requires corrections for atmospheric, angular and topographic effects. To do retrieval with TOC reflectance it is necessary to separate atmospheric correction and inversion, while the strong radiative coupling between surface and atmosphere makes this approach hard to justify. Although most attention has been given to the retrieval of vegetation biophysical and chemical characteristics from the TOC reflectance (Bacour et al., 2006; Baret et al., 2007; Combal et al., 2002; D'Urso et al., 2009; Goel, 1988; Goetz, 1997; Moreno et al., 2003; Schlerf and Atzberger, 2006; Tang et al., 2007), there are studies that highlight the advantages of a TOA radiance approach for variable retrieval (Laurent et al., 2011a; Mousivand et al., 2014; Verhoef and Bach, 2007).

Retrieval using TOA radiance has the advantage that no correction/conversion is necessary and the actual radiometric measurements can be used for retrieval. This is, in particular, important in the case of a multi-sensor retrieval approach (Mousivand et al., 2015a), where data acquired by sensors with different characteristics are integrated in the retrieval. Furthermore, the TOA retrieval approach would also allow retrieving surface and atmospheric properties simultaneously if spectral radiance measurements are sensitive to those properties.

Variable retrieval using TOA radiance data requires modeling of TOA radiance. Radiative transfer models explain the propagation of radiation through a medium (e.g. vegetation) and have been frequently and successfully used to simulate reflectance and radiance of soil-vegetation-atmosphere systems (Bacour et al., 2002; Jacquemoud et al., 2009; Verhoef and Bach, 2003a). TOA radiance modeling involves coupling radiative transfer models of surface and atmosphere. The radiance coming into the field of view of a sensor is the integrated sum of the surface reflectance, atmospheric effects and target's surroundings. Therefore, a careful modeling of each contribution is required to accurately calculate TOA radiance. A number of comprehensive simulation tools coupling surface and atmosphere radiative transfer models has been introduced (Borner et al., 2001; Fourty and Baret, 1997; Guanter and Kaufmann, 2009; Isaacs and Vogelmann, 1988; Kerekes and Landgrebe, 1989; Parente et al., 2010; Rahman et al., 1993b; Schott et al., 1999; Verhoef and Bach, 2003b, 2012; Zhang et al., 2010). However, some of these studies are often simplified through various assumptions such as flat terrain, Lambertian assumption for the surface reflectance and some other are more accurate but at very high computational cost that limits their application.

Among them, the four-stream approach proposed by Verhoef and Bach (2003b, 2007 and 2012) is a good example of a trade-off between computational efficiency and accuracy. It integrates the Soil-Leaf-Canopy radiative transfer model SLC with the atmospheric radiative transfer model MODTRAN. The approach has been validated against both synthetic and satellite data (Verhoef and Bach, 2007; Widlowski et al., 2007) and it has been used for the retrieval of vegetation properties over flat terrain (Laurent et al., 2011b, 2013; Mousivand et al., 2015a). Variable retrieval from TOA radiance over rugged terrain may need to account for topographic effects.

Topography has three major effects on the radiance sensed by a sensor. First, the total optical depth (gases and aerosols) decreases with increase in elevation. Second,

topography regulates the fraction of direct and diffuse irradiance received on a pixel from the sun and the sky respectively. Finally, topography changes the orientation of a target and therefore alters the illumination and viewing angles which affect reflected radiance because of the surface anisotropic reflectance. Topographic effects are determined by the aspect and slope of the surface and the local horizon, and also by the geometry of the surrounding areas (Gratton et al., 1993). The topographic effects can be as important as the atmospheric effects (Gonzalez-Sanpedro et al., 2008).

The four-stream approach is used for the simulation of TOA radiance. The approach was initially developed for flat terrain and it has been recently extended to account for sloped terrain as well (Verhoef and Bach, 2012). However, the extended approach only accounts for the slope and aspect of the observed pixel, while the topographic effects caused by the adjacent features (e.g. cast shadow and terrain reflected radiance) are not taken into account. A further concern is related to the extraction of the atmospheric coefficients in the four-stream approach. The atmospheric coefficients are derived from three MODTRAN runs at 0, 0.5 and 1 surface albedos with the assumption of Lambertian flat surface (Verhoef and Bach, 2003b, 2012). Apart from the computational burden of three calls to the code, the use of zero albedo may lead to some inconsistencies in some of the MODTRAN features (Guanter et al., 2009).

This study aims at addressing three issues: (i) investigating the effect of topography on TOA radiance, (ii) quantifying which slope and aspect requires integrated topography modeling, and; (iii) how does the topographic effect compare with the variability in TOA radiance due to variability of vegetation properties. In order to accomplish these goals, this paper presents an extension of the four-stream radiative transfer theory over heterogeneous non-Lambertian surfaces, in which topographic, adjacency and atmospheric effects are taken into account. Focus is given to the topography-induced contributions to the top of atmosphere radiance simulation. In this way, the impacts of topography on the irradiance and surface reflectance are precisely modelled using sky view factor and terrain reflected radiance from adjacent slopes. The surface reflectance at every location is modelled using SLC, while the atmosphere is modelled using MODTRAN. The MODTRAN Interrogation Technique (MIT) used for the extraction of atmospheric coefficients has been modified and reformulated to use only two MODTRAN runs instead of the three runs suggested in previous works and also to avoid the use of zero albedo in the calculation.

The remainder of the paper is structured as follows. Section 5.2 gives a detailed background of TOA radiance simulation using the four-stream theory. In Section 5.3, the extension of the four-stream theory over rugged terrain is described and topography effects on TOA radiance and surface reflectance are elaborated in details. The modified MODTRAN interrogation technique is also explained in Section 5.3. Section 5.4 describes the model implementation and the design of the numerical experiment is given in Section 5.5. The results of TOA radiance simulations considering different cases of rugged terrains are discussed in Section 5.6. Finally, Section 5.7 concludes the paper.

5.2. Background

The sensor reaching radiance is a complicated function of the interactions of solar radiation with the Earth's atmosphere and surface. Following Vermote et al. (1997), Ver-

hoef and Bach (2003b, 2007), and Schott (2007), the main paths through which radiation reaches the sensor over a flat surface are illustrated in Figure 5.1. Each contribution is briefly explained in Table 5.1.

Table 5.1: Different contributions in Figure 5.1 from the atmosphere and the surface to the sensor plus the corresponding fluxes in Figure 5.2

Contribution in Figure 5.1	Description	Corresponding flux in Figure 5.2
Contribution 1	spectral radiation originating from the sun and, after propagation in the atmosphere, scattered into the field of view of the sensor without reaching the surface.	$\rho_{so}E_s(t)$
Contribution 2	direct radiation that goes through the atmosphere without being absorbed or scattered and after reflecting back from the surface it reaches the sensor.	integrated in $\tau_{oo}E_o(b)$
Contribution 3	spectral radiation scattered by the atmosphere onto the target and then reflected back towards the sensor.	integrated in $\tau_{oo}E_o(b)$
Contribution 4&5	spectral radiation that directly or diffusely reach the surrounding areas of the target and then reflected or scattered back into the field of view of the sensor. This effect is so called “ <i>adjacency effect</i> ” or “ <i>blurring effect</i> ”.	$\tau_{do}E^+(b)$
Contribution 6	diffuse radiation coming from the adjacent features into the field of view of the sensor. This contribution is incorporated in Contribution 3.	—
Contribution 7	so-called trapping effect and it is a part of the radiation reflected from the surface into the air column above the surface being scattered and ultimately reaches the sensor. This contribution is incorporated in Contribution 3.	—

As shown in Figure 5.1, the top of atmosphere radiance over a non-Lambertian non-homogeneous Earth’s surface is determined by a combination of the surface reflectance, atmospheric effects, target’s surroundings effects and illumination and viewing geome-

try. This combination can be effectively modeled using the four-stream radiative transfer theory proposed by Verhoef and Bach (2003b, 2007, 2012). The four-stream approach is applied in this study. Figure 5.2 illustrates the relevant fluxes at the top and bottom of the atmosphere considered in the four-stream approach. At the top of the atmosphere, the only downward flux is assumed to be the direct solar irradiance and the only upward flux is the radiance in the direction of the sensor. At the bottom of the atmosphere, four different fluxes are considered; an attenuated direct solar flux (E_s); a surface radiance (times π) in the observation direction (E_o); diffuse downward flux from the sky ($E^-(b)$) and diffuse upward flux ($E^+(b)$) are considered. We follow the notations adopted by Verhoef and Bach (2003b, 2007, 2012) in this study as presented in Table 5.1.

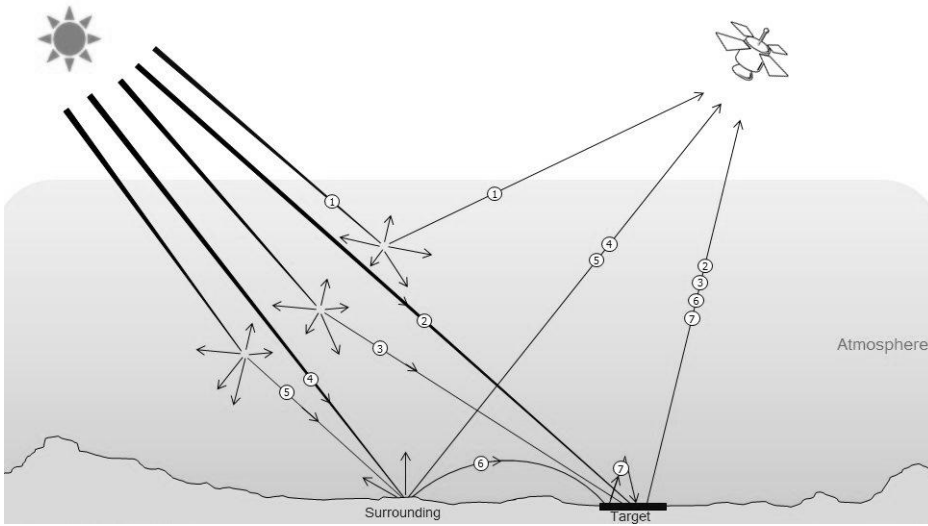


Figure 5.1: Various paths from the surface and the atmosphere to the TOA radiance

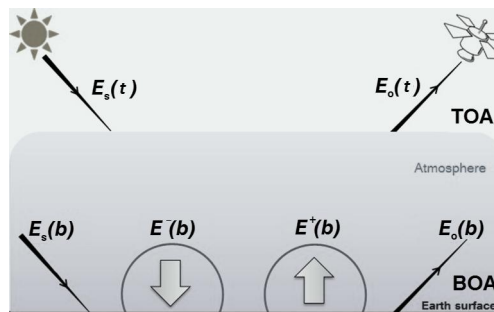


Figure 5.2: Four-stream radiation fluxes at the top (TOA) and the bottom (BOA) of the atmosphere; after (Verhoef and Bach, 2003b)

According to the four-stream theory, the TOA radiance in the direction of the sensor can be described as the sum of three components; the atmospherically scattered direct

solar radiation (atmospheric radiance); diffuse upwelling flux scattered into the direction of the sensor (adjacency effect) and the reflected radiance from the surface (target radiance), given by

$$E_o(t) = \rho_{so}E_s(t) + \tau_{do}E^+(b) + \tau_{oo}E_o(b) \quad (5.1)$$

where

$$E_s(b) = \tau_{ss}E_s(t) \quad (5.2)$$

$$E^-(b) = \tau_{sd}E_s(t) + \rho_{dd}E^+(b) \quad (5.3)$$

$$E^+(b) = \overline{r_{sd}}E_s(b) + \overline{r_{dd}}E^-(b) \quad (5.4)$$

$$E_o(b) = E_s(b)r_{so} + E^-(b)r_{do} \quad (5.5)$$

Eq 5.1 explains how the TOA radiance is generated from the sum of three components multiplied by atmospheric transmittance and hemispherical albedo. Eq 5.2 gives the attenuated direct solar flux at the bottom of the atmosphere, i.e. determined by the direct atmospheric transmittance from the sun to the ground. Eq 5.3 describes the diffuse downward flux (sky irradiance) by diffusely transmitted solar flux and upwelling diffuse flux from the surface that is reflected back by the atmosphere. Eq 5.4 describes the diffuse upward flux by the attenuated direct solar flux times the average surroundings diffuse reflectance and sky irradiance multiplied by the bi-hemispherical reflectance spatially averaged over surroundings. Finally, Eq 5.5 gives the surface radiance in the observation direction as a combination of the diffuse downward flux and the attenuated direct solar flux multiplied by hemispherical-directional reflectance and bidirectional reflectance respectively.

Natural surfaces usually exhibit anisotropic reflectance characteristics which describe the dependency of the reflectance spectra on the illumination and viewing geometry. This is defined by the Bidirectional Reflectance Distribution Function (BRDF). The BRDF of vegetation canopies can be described by canopy radiative transfer models, i.e. SLC in this study. To properly model the radiative interactions between the surface and atmosphere, complete BRDF functions are required, which means three or four dimensional functions depending on the undertaken assumption of azimuthal symmetry (Verhoef and Bach, 2003b). The anisotropic reflectance patterns of vegetated surfaces in a non-Lambertian approach has to be described by a minimum of four reflectance factors (Verhoef and Bach, 2003b). In this study, the four directional reflectance factors; r_{so} , r_{do} , r_{sd} and r_{dd} calculated by the SLC describe the anisotropic reflectance and can, therefore, be used to determine radiance reflected in any direction of observation, given the irradiance and the direction of illumination.

By substituting different equations in Eq 5.1 and solving the diffuse fluxes at the surface, the TOA radiance can be obtained (Verhoef and Bach, 2003b)

$$L_{TOA} = \frac{E_s^o \cos(\theta)}{\pi} \left[\underbrace{\rho_{so}}_{\text{atmosphere}} + \underbrace{\frac{\tau_{ss}\overline{r_{sd}} + \tau_{sd}\overline{r_{dd}}}{1 - \overline{r_{dd}}\rho_{dd}}}_{\text{adjacency}} \tau_{do} + \underbrace{\tau_{ss}r_{so}\tau_{oo}}_{\text{sun}} + \underbrace{\frac{\tau_{sd} + \tau_{ss}\overline{r_{sd}}\rho_{dd}}{1 - \overline{r_{dd}}\rho_{dd}}}_{\text{sky}} r_{do}\tau_{oo} \right] \quad (5.6)$$

Four surface reflectance factors plus six atmospheric coefficients are required in the four-stream approach to model TOA radiance (see Table 5.2 for definitions). The surface reflectance components are described by the SLC radiative transfer model (Verhoef and Bach, 2003b) and the atmospheric coefficients are derived from the MODTRAN4 atmospheric radiative transfer model. There is no term in Eq 5.6 to account for the topography effects. Verhoef and Bach (2012) proposed an extension of Eq 5.6, in which topography effects are considered. The proposed approach, however, does not fully account for topographic impacts, since only the slope and aspect of the observed pixel itself are taken into account, while the obstructing effects of neighboring facets are not.

Table 5.2: Terminology used in the study (after Verhoef & Bach, 2003b, 2007 and 2012)

Factor	Description	SI unit
r_{so}	surface bidirectional reflectance factor	[-]
r_{do}	surface hemispherical-directional reflectance for diffuse incidence	[-]
$\overline{r_{sd}}$	spatially averaged directional-hemispherical reflectance over surroundings	[-]
$\overline{r_{dd}}$	spatially averaged bi-hemispherical reflectance over surroundings	[-]
ρ_{so}	TOA atmospheric bidirectional reflectance	[-]
ρ_{dd}	BOA spherical albedo of the atmosphere	[-]
τ_{ss}	direct atmospheric transmittance from the sun to the ground	[-]
τ_{oo}	direct atmospheric transmittance from the ground to the sensor	[-]
τ_{sd}	diffuse atmospheric transmittance from the sun to the ground	[-]
τ_{do}	diffuse atmospheric transmittance from the ground to the sensor	[-]
E_s^o	extraterrestrial solar irradiance on a plane perpendicular to the sunrays	Wm^{-2}
E_s	direct solar irradiance on a horizontal plane	$Wm^{-2}\mu m^{-1}$
E_o	radiance in the viewing direction, times π	$Wm^{-2}\mu m^{-1}$
E^-	downward diffuse irradiance	$Wm^{-2}\mu m^{-1}$
E^+	upward diffuse irradiance	$Wm^{-2}\mu m^{-1}$
ξ	binary coefficient to indicate cast-shadowed pixels (0 or 1)	[-]
θ_s	local solar zenith angle	degree
θ_o	viewing zenith angle	degree
i	angle between the surface normal and the sun ray (illumination angle)	degree
β	surface slope angle	degree
φ_s	solar azimuth angle	degree
φ_t	slope azimuth angle (aspect)	degree
t	indicates the quantity at the top of atmosphere	[-]
b	indicates the quantity at the bottom of atmosphere	[-]

5.3. Four-stream theory over rugged terrain

In this section, we present an extension of the four-stream theory with the focus on modeling the topography-induced effects on the TOA radiance. Accordingly, Eq 5.1 will have

to be modified to account for the topography effects. Among different terms in this equation, the reflected radiance from the surface ($\tau_{oo}E_o(b)$) is directly related to the surface topography and to the anisotropy of surface reflectance. In this way, we reformulate $E_o(b)$ to include both the diffuse downward flux and the attenuated direct flux to consider topography effects.

5.3.1. Irradiance modeling

The total solar irradiance reaching the ground surface on an inclined surface can be expressed as the sum of direct, diffuse and terrain irradiance components. Figure 5.3 depicts the contribution of different components to the incoming irradiance on an inclined surface. The ratio of direct and diffuse fluxes is a function of the surface orientation, elevation and shadows cast by topographic features (Sandmeier and Itten, 1997). A Digital Elevation Model (DEM) is required to model topography effects on irradiance. Multiplying the irradiance components by the relevant non-Lambertian surface reflectance factors will give the total outgoing radiance from an inclined surface headed toward the sensor in the four-stream approach. We express the total surface reflected radiance in the observation direction as the sum of the direct ($E_{o_{dir}}(b)$), diffuse ($E_{o_{diff}}(b)$) and terrain ($E_{o_{terr}}(b)$) radiance components;

$$E_o(b) = E_{o_{dir}}(b) + E_{o_{diff}}(b) + E_{o_{terr}}(b) \quad (5.7)$$

In the following sections, we elaborate on each of these components and discuss how they will interact with different upward and downward fluxes.

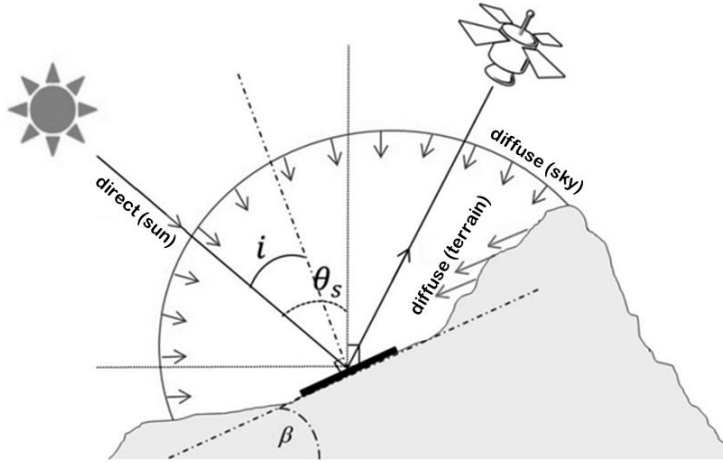


Figure 5.3: Contributions of irradiance on an inclined surface; direct, diffuse and terrain irradiances

Direct irradiance: The direct irradiance is the main contribution to the total solar irradiance under clear sky conditions. This component depends on target's elevation (which is considered in the atmospheric radiative transfer model), sun-target geometry and the horizon profile that determines shadow distribution. The direct irradiance

multiplied by the bidirectional reflectance factor (r_{so}) of the surface yields the direct radiance at the ground level reflected towards the sensor.

$$E_{o_{dir}}(b) = \xi E_s(b) \frac{\cos i}{\cos \theta_s} r_{so} \quad (5.8)$$

where $\cos i = \cos \theta_s \cos \beta + \sin \theta_s \sin \beta \cos(\varphi_s - \varphi_t)$. If $\cos i$ is negative, the pixel is self-shadowed and does not receive direct radiation. A pixel may also be cast-shadowed when the direct path between the pixel and the sun is intercepted by another terrain feature. This binary factor ξ (0 or 1) indicates whether the pixel is cast-shadowed by adjacent features (Dozier et al., 1981).

Diffuse irradiance: The diffuse (or sky) irradiance includes two components; short-wave diffuse radiation scattered by various atmospheric constituents and longwave atmospheric emittance (Gratton et al., 1993). The latter is not considered in this study as we only account for the shortwave component. The diffuse irradiance is a function of the proportion of sky that is visible from the pixel. A simple assumption is to assume that this quantity is isotropic over the entire sky hemisphere. However, in reality, this quantity exhibits some anisotropic behavior, especially when the slope is greater than 20 degree (Proy et al., 1989), and a more realistic estimate would be to decompose it into isotropic and anisotropic circumsolar components. The ratio of isotropic and anisotropic components can be derived by means of Hay (1993) “anisotropy index” (k). The index k is defined as the ratio of circumsolar diffuse irradiance to the total sky diffuse irradiance. The direct atmospheric transmittance along the sun-target path is used to define this index (Hay, 1993) such that $k = \frac{B_n}{I_0} \approx \tau_{ss}$, B_n where denotes the beam radiation on a surface normal to the solar ray and I_0 is the extraterrestrial solar constant. In atmospheric radiative transfer models, this index is simply the direct transmittance from the sun to the ground. The diffuse irradiance multiplied by the hemispherical-directional reflectance factor (r_{do}) of the surface gives the diffuse radiance at the ground level reflected towards the sensor.

$$E_{o_{diff}}(b) = E^-(b) \left[\underbrace{k \frac{\cos i}{\cos \theta_s}}_{\text{anisotropic}} + \underbrace{(1-k) V_{sky}}_{\text{isotropic}} \right] r_{do} \quad (5.9)$$

The factor V_{sky} , known as sky view factor (Figure 5.4 left), is defined as the relative proportion of the solid angle of the sky which is seen from a pixel and is not blocked by the surrounding topography (range between 0 and 1). The most widely used method is the simple trigonometric approximation presented in Liu and Jordan (1960) and many others:

$$V_{sky} = \frac{1 + \cos \beta}{2} \quad (5.10)$$

This expression is not in accordance with the definition of the sky view factor and does not represent it properly (Rakovec and Zaksek, 2012). The only variable is the slope angle of the surface itself and the obstructing effects of surrounding topography are not considered. For an infinitely long slant surface or semi-rugged areas this would not lead

to significant errors in the calculations, but over rugged terrain the effect of the surrounding topography plays an important role and must be taken into account as well. To account for this effect, the algorithm proposed by Dozier et al (1981, 1990) is applied in this study that provides a more accurate and analytical approximation of the sky view factor and is computationally efficient. The algorithm searches around the target for features high enough to obstruct the sun. This has to be done over the entire azimuthal range. However, in practice, a specified number of directions () over the range $0 \leq \theta \leq \pi$ (e.g. 16 directions) are taken to determine the horizon angles for the complete circle (Dozier and Frew, 1990). The horizon can result either from "self-shadowing" or from adjacent ridges. Horizon angles are interpolated for all other unsearched directions. Then, the sky view factor is calculated by integrating the horizon angles over the azimuth circle.

$$V_{sky} = \frac{1}{\pi} \int_0^{2\pi} \int_0^{h_{\phi i}} \sin \theta [\cos \theta \cos \beta + \sin \theta \sin \beta \cos (\phi - \phi_i)] d\theta d\phi \quad (5.11)$$

If N is the number of discrete set of directions over the entire circle and $h_{\phi i}$ represents the horizon angle in direction i , then

$$V_{sky} \approx \frac{1}{N} \sum_{i=1}^N \cos \beta \sin^2 h_{\phi i} + \sin \beta \cos (\phi_i - \phi) (h_{\phi i} - \sin h_{\phi i} \cos h_{\phi i}) \quad (5.12)$$

The sky view factor is an intrinsic characteristic of topography and does not considerably change over time. It is, therefore, adequate to compute this factor once at high azimuthal resolution (i.e. for a large number of directions) before the simulation. In this study, we calculated the sky view factor at each pixel for 64 azimuth directions.

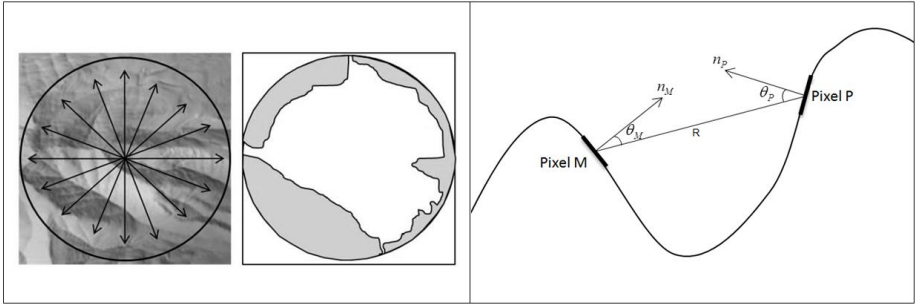


Figure 5.4: An example of sky view factor (left) and terrain irradiance from pixel P into pixel M (right)

Terrain irradiance: In rugged terrains, apart from the diffuse radiation from the sky dome, the adjacent slopes visible from the pixel will also contribute to the irradiance reaching the pixel. This component is often considered to be relatively insignificant and is neglected in most studies (Gratton et al., 1993; Proy et al., 1989). However, if the surface's cover is highly reflective (e.g. snow and ice) or in mountainous areas with deep valleys, it is important to estimate this component. As an example, Gratton et al. (1993)

showed that in a glacier basin between 10% to 25% of the total irradiance at any location was terrain irradiance for non-shadowed and large shadowed areas.

An accurate method to calculate irradiance from the adjacent terrain was used in Proy et al.(1989). We hereafter refer to this as the exact method. The method calculates the sum of the radiance coming from all the pixels that are seen from any observed pixel. The terrain irradiance at a pixel M , coming from pixel P is given by:

$$E_{terr} = \sum_{i=1}^N \frac{\cos T_M \cos T_P dS_M dS_P}{R^2} E_o^P(b) \quad (5.13)$$

where $\cos T_M$ and $\cos T_P$ are the angles between normal and the line that connects two pixels (Figure 5.4 right), dS_P and dS_P are the area of pixels P and M , R is the distance between the pixels, N is the number of visible pixels from M and $E_o^P(b)$ is the total radiance of pixel P coming towards pixel M that can be calculated using Eq 5.7. However, there is a challenge in accurately determining the total radiance coming from pixel P , since at the same time $E_o^P(b)$ is both the input for terrain irradiance (Eq 5.13) and the output in Eq 5.7. The solution applied in this study was to ignore the terrain irradiance in the first iteration and calculate $E_o^P(b)$ from the sum of the direct and diffuse terms considering the geometry relationship between pixels M and P , and then iterate this procedure to account for the terrain irradiance as well. The attenuation of the radiance between two pixels is ignored. The effective distance from which the radiance of neighboring pixels arrives at the observed pixel can be considered between 0.5 to 1 km (Richter, 1998), which in this study we have considered a radius of 1 km from the observed pixel. The exact method is computationally intensive and it is often replaced by an approximation. In this case, the portion of the surrounding pixels seen from the observed pixel (known as terrain view factor) is estimated by a simple trigonometric approximation,

$$V_{terrain} \approx \frac{1 + \cos \beta}{2} - V_{sky} \quad (5.14)$$

Then, the average radiance scattered off the neighboring areas within the horizon of the observed pixel is multiplied by the terrain view factor to get an approximation of the terrain irradiance at the observed pixel.

The integration of radiance contribution of different components leads to;

$$E_o(b) = \underbrace{\xi E_s(b) \frac{\cos i}{\cos \theta_s} r_{so}}_{direct} + \underbrace{E^-(b) \left[\tau_{ss} \frac{\cos i}{\cos \theta_s} + (1 - \tau_{ss}) V_{sky} \right] r_{do}}_{diffuse} + \underbrace{E_{terr} r_{do}}_{terrain} \quad (5.15)$$

This equation describes the reflected radiance by a non-Lambertian, non-homogeneous rugged terrain at the bottom of the atmosphere. Modeling of the non-Lambertian reflectance is described below. Since terrain-related quantities (e.g. sky view, terrain view, slope, and aspect) are spectrally independent, they can be considered as multiplicative constants. Accordingly, we define the terms below;

$$F_{sun} = \xi \frac{\cos i}{\cos \theta_s}; F_{sky} = \tau_{ss} \frac{\cos i}{\cos \theta_s} + (1 - \tau_{ss}) V_{sky}$$

Therefore, Eq 5.5 on sloped terrain turns into;

$$E_o(b) = F_{sun}E_s(b)r_{so} + F_{sky}E^-(b)r_{do} + E_{terr}r_{do} \quad (5.16)$$

It has to be noted that the spatial resolution of the DEM plays a crucial role in the estimation of the topography effects. To accurately estimate these effects, a DEM of a resolution equal to or higher than the sensor's spatial resolution is required (Richter and Schlapfer, 2002).

5.3.2. Reflectance modeling

Topography influences the orientation of surface and hence alters the illumination and viewing angles of the observed pixels. Apart from the bi-hemispherical reflectance (r_{dd}), the other three reflectance factors calculated by the SLC determine additional changes in the reflected radiance depending on the illumination and viewing geometry. To account for surface anisotropic reflectance effect, the SLC calculations have to be done with the illumination and viewing angles considering the topography effect on the orientation. This effect is also considered in the estimation of terrain irradiance from one pixel to another, as described above. It has to be noted that leaves tend to maintain their LIDF with respect to the gravity field, so in principle the BRDF would stay invariant, but in the case of sloped terrain photon paths inside the vegetation layer change compared to those for a flat terrain case, so some effect on the BRDF is expected. However, this has not been considered in this study.

5.3.3. Top of atmosphere radiance over rugged terrain

By substituting Eq 5.16 in Eq 5.1 and solving the diffuse fluxes at the surface, the TOA radiance over rugged terrain is obtained by

$$L_{TOA} = \frac{E_s^o \cos \theta}{\pi} \left[\underbrace{\rho_{so}}_{\text{atmosphere}} + \underbrace{\frac{\tau_{ss}\tau_{sd} + \tau_{sd}\tau_{dd}}{1 - \tau_{dd}\rho_{dd}}\tau_{do}}_{\text{adjacency}} + \underbrace{\tau_{ss}\tau_{so}\tau_{oo}F_{sun}}_{\text{sun}} + \underbrace{\frac{\tau_{sd} + \tau_{ss}\tau_{sd}\rho_{dd}}{1 - \tau_{dd}\rho_{dd}}\tau_{do}\tau_{oo}F_{sky}}_{\text{sky}} + \underbrace{E_{terr}\tau_{do}\tau_{oo}}_{\text{terrain}} \right] \quad (5.17)$$

The definitions of different terms are given in Table 5.2. The multiplicative factor $1 - \tau_{dd}\rho_{dd}$ in the equations above accounts for multiple reflections between the surface and the atmosphere (Rahman et al., 1993b). Also, the spatial filtering kernel of the adjacency effect is defined by $\overline{\tau_{dd}} = \frac{1}{n^2} \sum_{i=1}^n r_{dd}$ where n is the number of pixels for the area taken for adjacency effect ($\approx 1\text{ km}$ in this study). However, due to the fact that the scattered photons are spread over a much larger region when the deflection angle increases and due to the strong forward scattering of aerosols, the required filtering kernel should be sharply peaked in the center. Moreover, this filtering kernel would give an approximation of the adjacency effect in the case of sloped terrain since the mean reflectance τ_{dd} will depend on other factors as well, such as the orientation of adjacent terrain facets. Additionally, the atmospheric reflectance ρ_{so} in Eq 5.17 may change according to the local topography which in that case it requires pixel-wise modeling of the atmosphere. In this study, we have assumed a constant atmosphere over the study area and hence ρ_{so} is assumed to be constant across the study area.

In order to calculate TOA radiance, the unknown parameters in Eq 5.17 have to be determined. Amongst the parameters in the equation, four surface reflectance factors are calculated for a given surface with known properties (soil, leaf and canopy properties) on a pixel-by-pixel basis from the SLC model (see § 5.3.2). In case of rugged terrain a DEM is applied to derive slope, aspect, sky view factor and terrain view factors to estimate topography-induced effects (see § 5.3.1). In fact, for a specified scenario only atmospheric coefficients have to be determined. Six atmospheric coefficients plus extraterrestrial solar irradiance are determined by applying an atmospheric radiative transfer code like MODTRAN (Berk et al., 2003, 1998). In this study MODTRAN4 was used to calculate the atmospheric coefficients. We implemented a modified version of the MODTRAN interrogation technique (Verhoef and Bach, 2003b, 2007) to estimate atmospheric coefficients. We briefly explain MODTRAN and then the modified MIT approach is given in more detail in the next Section.

5.3.4. Atmospheric modeling

Modified MODTRAN Interrogation Technique (MIT)

MODTRAN (MODerate resolution atmospheric TRANsmittance and radiance code) was initially developed from the LOW resolution TRANsmittance 7 (LOWTRAN 7) radiative transfer model. It models radiation scattering and absorption through the atmosphere. Atmospheric multiple scattering is computed using the scaled *DISORT* (DIScrete Ordinate Radiative Transfer) algorithm and the correlated *k* algorithm is used to model the absorption for regions presenting considerable absorption effects. MODTRAN allows flexibility in the input parameters where both user inputs and predefined profiles for different atmospheric scenarios are accepted. MODTRAN has been successfully used for both at sensor radiance simulation (Laurent et al., 2011b; Mousivand et al., 2015a; Schlapfer and Nieke, 2005; Verhoef and Bach, 2003b, 2007, 2012) and for atmospheric correction (Adler et al., 1999; Schlapfer and Richter, 2002) from the visible to the thermal infrared wavelength region. The computational cost of a MODTRAN run is dependent on the calculation mode, as well as whether using DISORT with various streams. MODTRAN takes an ASCII file (with **.tp5* suffix) as input and delivers some standard output files, while the files with suffix *"*.tp7"* and *"*.7sc"* are of interest for use in the simulation procedure. The standard MODTRAN outputs do not directly provide the unknown atmospheric coefficients required in the four streams RT approach and they have to be computed from such outputs. Table 5.3 lists the standard MODTRAN4 outputs along with formulas and explanation of each column.

Verhoef and Bach (2003b, 2012) have shown that the six atmospheric coefficients in Eq 5.17 can be derived from three MODTRAN runs for surface albedos at 0, 0.5 and 1 using the so-called MODTRAN Interrogation Technique (MIT). These runs are done assuming uniform Lambertian surface reflectance, given atmospheric state and angular configuration. We have modified the algebra used by Verhoef and Bach (2003b, 2012) to improve computational efficiency. In the modified MIT, only two MODTRAN runs are required to extract the atmospheric coefficients. The two runs can be with any spectrally flat surface albedos between 0 and 1. It is recommended to avoid using zero albedo since it leads to some miscalculations in the extracted parameters from MODTRAN (Guanter et al., 2009). For instance, with a black surface assumption, the scaling in the scaled-

Table 5.3: Standard MODTRAN outputs with the given headers, column number, formula and relevant descriptions

MODTRAN(*.tp7 or *.7sc)	Column	Formula	Description
FREQ	1	—	band-center wavelength
TRAN	2	τ_{oo}	direct transmittance from the ground to the sensor
PTH THRML	3	—	upwelling atmospheric emitted radiance received at the sensor(Negligible in the reflective region)
THRML SCT	4	—	thermal scattering of the path radiance
SURF EMIS	5	—	surface emission received at the sensor
SOL SCAT	6	$\frac{E_s^0 \mu_s}{\pi} \left[\rho_{so} + \frac{(\tau_{ss} + \tau_{sd})}{1 - a\rho_{dd}} a\tau_{do} \right]$	solar multi-scattered radiance received at the sensor(PATH)
SING SCAT	7	—	solar single-scattered radiance
GRND RFLT	8	$\frac{E_s^0 \mu_s}{\pi} \left[\frac{(\tau_{ss} + \tau_{sd})}{1 - a\rho_{dd}} a\tau_{oo} \right]$	ground reflected radiance (GRT)
DRCT RFLT	9	$\frac{E_s^0 \mu_s}{\pi} [\tau_{ss} a\tau_{oo}]$	direct solar reflected radiance received at the sensor(GSUN)
TOTAL RAD	10	TOTAL RAD = SOL SCAT + GRND RFLT	PTH THRML + SURF EMIS + SOL SCAT + GRND RFLT (GTOT)
REF SOL	11	$E_s^0 \tau_{ss} \tau_{oo}$	SOL@OBS multiplied by $\tau_{ss} \tau_{oo}$
SOL@OBS	12	E_s^0	extraterrestrial solar irradiance
DEPTH	13	$b = -\ln(\tau_{oo})$	negative Log of the transmittance column TRAN (total optical thickness)

DISORT option by MODTRAN is not applied over the diffuse fluxes, which results in miscalculation of the spherical albedo parameter. We have used two different spectrally flat surface albedos, i.e. 0.5 and 1. The modified MIT needs the solar-scattered path radiance (SOL SCAT in Table 5.3 and the total ground-reflected radiance contribution (GRND RFLT in Table 5.3) for surface albedos at 0.5 and 1 plus the radiance contribution due to ground-reflected sunlight (DRCT RFLT in Table 5.3) for surface albedo at 1.

If we assume a uniform Lambertian surface reflectance with albedo a , the TOA radiance signal in Eq 5.17 turns into the simplified equation

$$L_{TOA} = \underbrace{\frac{E_s^o \mu_s}{\pi} \left[\rho_{so} + \frac{(\tau_{ss} + \tau_{sd})}{1 - a\rho_{dd}} a\tau_{do} \right]}_{PATH} + \underbrace{\frac{E_s^o \mu_s}{\pi} [\tau_{ss} a\tau_{oo}]}_{GSUN} + \underbrace{\frac{E_s^o \mu_s}{\pi} \left[\frac{(\tau_{ss} a\rho_{dd} + \tau_{sd})}{1 - a\rho_{dd}} a\tau_{oo} \right]}_{GSKY} \quad (5.18)$$

Here, GSKY stands for the radiance contribution due to sky irradiance in the direction of viewing. We first extract τ_{ss} by substituting τ_{oo} and E_s^o (direct outputs from TRAN and SOL@OBS in Table 5.3) into GSUN for surface albedo at 1,

$$\tau_{ss} = \frac{GSUN_1 \times \pi}{E_s^o \mu_s \times \tau_{oo}} \quad (5.19)$$

It should be noted that, as shown in Verhoef and Bach (2012), some equations in Table 5.3 are inaccurate in absorption bands of the atmosphere due to finite band width. For accurate applications one needs to make 2 runs at TOA and 2 at BOA, especially if an accurate surface irradiance is needed.

Next, the spherical albedo ρ_{dd} is computed from the combination of two GRT for surface albedos at 0.5 and 1,

$$\rho_{dd} = \frac{GRT_1 - 2 \times GRT_{0.5}}{GRT_1 - GRT_{0.5}} \quad (5.20)$$

Once ρ_{dd} and τ_{ss} are estimated, τ_{sd} can be derived from

$$\tau_{sd} = \left[\frac{GRT_1 (1 - \rho_{dd})}{GSUN_1} - 1 \right] \tau_{ss} \quad (5.21)$$

The diffuse atmospheric transmittance from the ground to the sensor τ_{do} can also be derived from the combination of two sets of PATH and GRT for surface albedos at 0.5 and 1

$$\tau_{do} = \left[\frac{PATH_1 - PATH_{0.5}}{GRT_1 - GRT_{0.5}} \right] \tau_{oo} \quad (5.22)$$

Finally, the atmospheric bidirectional reflectance ρ_{so} is derived using PATH and GRT for surface albedo at 1,

$$\rho_{so} = \left[PATH_1 - \left(\frac{GRT_1 \times \tau_{do}}{\tau_{oo}} \right) \right] \frac{\pi}{E_s^o \mu_s} \quad (5.23)$$

Therefore, for a given atmosphere and a known sun-target-sensor geometry all the six atmospheric coefficients are derived in this way. These atmospheric coefficients are spectrally dependent and as a common practice they can be assumed constant for an image due to the homogeneity of the atmosphere over small areas. It is more realistic, however, to model the atmospheric effects on a pixel wise manner (e.g. in a variable retrieval procedure) because of the high spatial variability of water vapor and aerosols. In that case, instead of direct calls to the atmospheric model, an alternative is to build up a large look up table where all the expected input combinations are covered. The computational cost of creating such look up tables is high and can be reduced using the modified MIT method.

5.4. Model implementation

TOA radiance over rugged terrain can be modeled using Eq 5.17. The unknowns in this equation are defined in Table 5.2 and we explain here how to determine such unknowns in this section.

First, the topography related factors are derived from the DEM including the slope, aspect, sky view factor and the list of pixels that are seen from each pixel. Second, sun and observer zenith and azimuth angles are calculated per pixel using the slope and aspect maps and the binary factor ξ is estimated as well. Third, for a given surface with known soil, leaf and canopy properties, the four canopy directional reflectance factors; r_{so} , r_{do} , r_{sd} and r_{dd} are calculated using the SLC per pixel considering the local sun and observer zenith angles and the relative azimuth angle. The spatial filtering kernel of the adjacency effect is then applied to the directional-hemispherical and the bi-hemispherical reflectance factors to obtain $\overline{r_{sd}}$ and $\overline{r_{dd}}$ in Eq 5.17 considering a radius of 1 km around the target pixel. Fourth, the atmospheric coefficients are derived from two MODTRAN4 runs using the modified MIT. The relevant equations (Eq 5.19 to Eq 5.23) to derive such coefficients are given in § 5.3.4. The next step is to estimate the factors F_{sun} and F_{sky} as well as E_{terr} using the equations in § 5.3.1. In this study, we calculate all the wavelength dependent factors at intervals of 1 nm and the calculated spectral radiance is later convolved with the sensor spectral response functions to generate sensor-specific radiometric data.

5

5.5. Design of the numerical experiment

To illustrate the effect of topography on the surface reflectance and TOA radiance, we have compared two scenes generated with SLC: the first one for the actual, flat-case, site of Barrax and the second one generated using exactly the same spatial patterns of vegetation, soil and atmospheric properties, but laid over the DEM of a mountainous area. The observations and ground truth data collected during the ESA SEN3EXP field campaign were used for this study. The eld campaign was carried out at the Barrax (N39°3', W2°60') test site and surrounding area from 20 to 24th of June 2009 as part of the development process for ESA's Sentinel-3 Earth observation mission (Brockmann et al., 2011). Barrax is an agricultural test site located in southeastern Spain on the La Mancha plateau characterized by relatively heterogeneous landscape with large uniform irrigated agricultural fields and rain-fed crops. The area consists of irrigated fields, harvested fields and bare soil which provide an appropriate environment for simulating heterogeneous anisotropic surface behavior. The DEM was taken from a mountainous region in the Austrian Alps. The elevation varies between 457 and 1526 meters with an average slope of 24° including both north-facing and south-facing hill slopes. Figure 5.5 (top row) shows the slope and aspect maps of the rugged surface used for this study. The aspect angle is referenced from the north.

This experimental design allows for a correct evaluation of the topographic effects, since we can compare the TOA radiance of the flat case with the rugged case for the same land-cover and the same atmosphere. The spatial information on soil, leaf and canopy properties were derived from an input TOA radiance CHRIS-Proba image of 19-06-2009 over the Barrax area (flat case) as explained in Mousivand et al. (2015a). The surface re-

flectance factors were calculated from the soil, leaf and canopy properties using the SLC model considering the local illumination and view directions (see § 5.3.2). The atmospheric coefficients were derived by applying the modified MIT using two MODTRAN runs. Next, having taken into account the topographic effects on the irradiance, the TOA radiance is calculated for the entire synthetic scene (rugged case). The effects of sky view factor, terrain view factor and solar illumination are then evaluated by comparing the actual scene for the flat case with the synthetic scene for the rugged case.

5.6. Results and discussion

5.6.1. Topography effects on the TOA radiance

Figure 5.5 (bottom row) shows the simulated TOA radiance CHRIS-Proba image (flat case, bottom left) and the simulated TOA radiance image over the rugged terrain (rugged case, bottom right). Visually comparing the images, the effect of higher irradiance on south facing facets is very clear, as well as the lower irradiance on north facing facets. For instance, Figure 5.6 (left) presents a rugged-case self-shadowed pixel (labeled “B” in Figure 5.5) with slope of 42° and aspect of 319° compared with the same flat-case pixel, while the right hand figure presents a pixel exposed to the sun (labeled “A” in Figure 5.5) with slope of 20° and aspect of 111° . In the left-hand figure, the self-shadowed pixel (blue) receives most irradiance from diffuse radiation causing lower reflected radiance, while the right-hand figure indicates the extra irradiance coming into the pixel due to the sun position and the topographic effects of neighboring areas. The full flat- and rugged-case scenes were compared and the result is illustrated by Figure 5.7, where the Root Mean Squared Difference (RMSD) values between the simulated flat- and rugged-case scenes are shown versus the slope and aspect angles. A positive correlation is seen between slope, aspect and RMSD. The smaller RMSD are attributed to areas with small slope and aspect characterizing flat areas and the RMSD increase with an increase in the slope and aspect. A considerable difference in RMSD is seen over north facing slopes even for intermediate slopes.

The illustrations above document to the impact of topography on TOA radiance. Apart from the general impact of topography, it is also interesting to check how sky view and terrain reflected radiance influence the TOA radiance. In the following sections we quantify the effect of these factors on the TOA radiance.

5.6.2. Sky view factor effect

In order to investigate the impact of sky view factor on TOA radiance, two different methods were used to calculate the sky view factor. Figure 5.8 (left and middle) displays the sky view factor calculated using the horizon (i.e. Eq 5.12) and the approximate (i.e. Eq 5.10) methods. The mean difference between the sky view factors calculated with the two methods is around 0.04. Considerable differences are seen (Figure 5.8 right), however, in the valleys and steep slopes (up to 0.30 difference). The approximate method generally overestimates the sky view factor due to the neglected effect of the neighboring areas.

We conducted two experiments to study the effect of sky view factor on the output radiance. We first simulated TOA radiance without applying sky view factor and second,

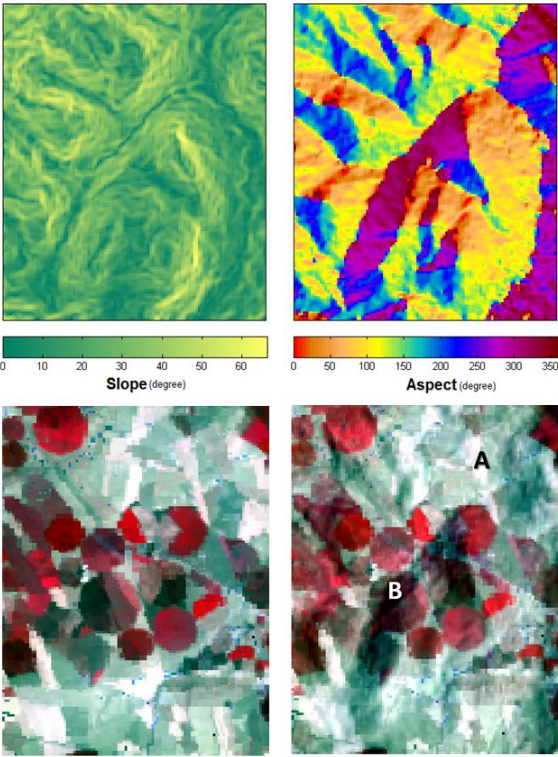


Figure 5.5: Top row: The slope (left) and aspect (right) maps used for generating the rugged terrain surface, Bottom row: RGB (870, 670 and 540 nm) band combination of the simulated CHRIS-Proba image flat-case (left) and over rugged terrain (right). The letters represent two pixels: “A” (a pixel exposed to the sun) and “B” (a self-shadowed pixel) (see § 5.6.1 for explanation)

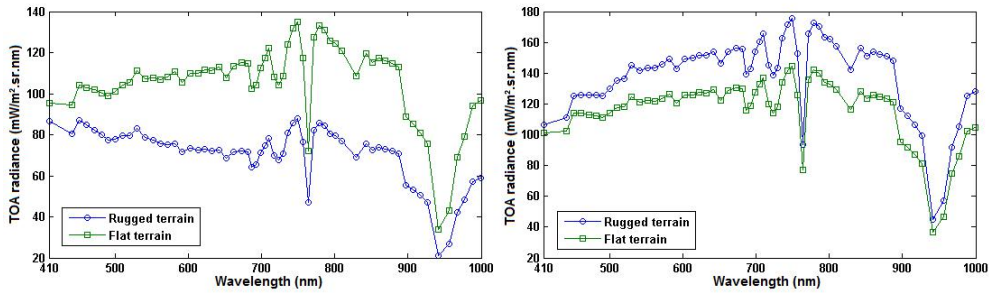


Figure 5.6: Comparison of the simulated TOA radiances over rugged terrain versus flat-case image for a self-shadowed pixel (left) and a pixel exposed to the sun (right)

we compared simulated TOA radiances applying two different sky view factors. All the other effects were kept identical for both cases and only in the second case the method to calculate the sky view factor from the DEM was changed.

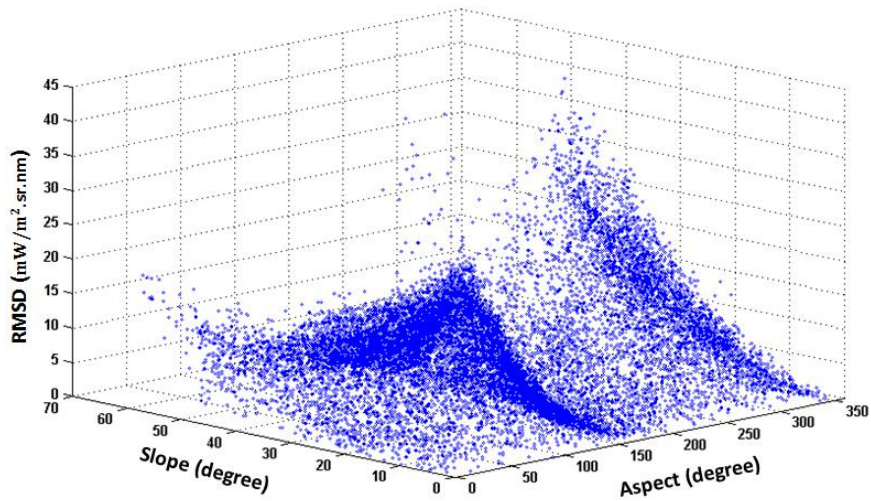


Figure 5.7: RMSD values between the simulated and actual images versus slope and aspect angles of the study area

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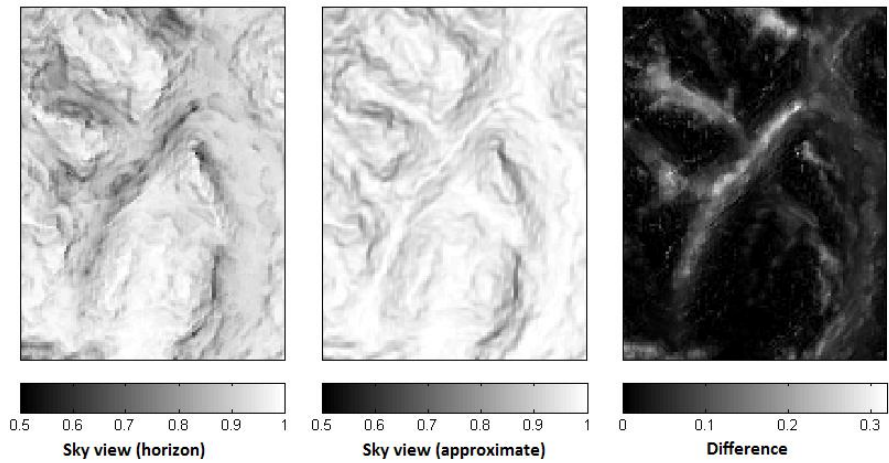


Figure 5.8: Sky view factor calculated using the horizon (left) and approximate (middle) methods and the difference (right) between the two methods

Figure 5.9 (left) illustrates the RMSD of all the CHRIS-Proba bands between the simulated radiance with and without applying sky view factor. RMSD values range from zero to 5 ($mW/m^2.sr.nm$), though the increasing discrepancy is attributed to the steep and north-facing slopes. This quantifies the effect of sky view factor on the output radiance and shows that neglecting this factor can cause considerable uncertainty in forward TOA radiance modeling in particular for steep slopes.

The RMSD between simulated TOA radiance using different sky view factors is shown

in Figure 5.9 (right). A maximum RMSD of 0.8 ($mW/m^2.sr.nm$) is seen in this case over north facing and steep slopes. Although, the RMSD are small in this case compared to the case when neglecting sky view factor, it still introduces uncertainty in the forward TOA radiance modeling. These results suggest that a precise estimation of the sky view factor is therefore essential to reduce the uncertainty in the TOA radiance modeling over rugged terrain. Therefore, the horizon method is recommended for the calculation of the sky view factor because of its fast calculation and also more accurate results than the approximate method.

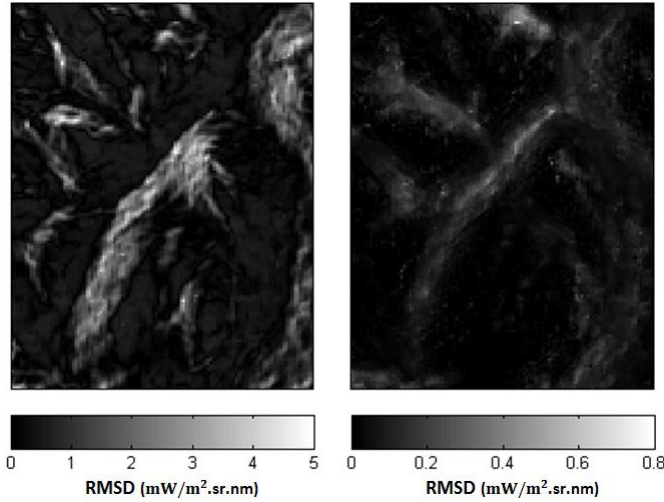


Figure 5.9: RMSD between simulated TOA radiance with and without applying sky view factor (left) and RMSD between simulated TOA radiance applying two different sky view factors (right)

5.6.3. Terrain reflected radiance effect

Terrain reflected radiance from adjacent slopes has been reported to have non-negligible impact on the TOA radiance in rugged terrain. To quantify the influence of this factor, we have calculated this contribution using two different approaches, the trigonometric approximation (i.e. Eq 5.14) and the exact calculation of the radiance reflected by adjacent pixels (Eq 5.13). We then compared the simulated TOA radiance without applying the terrain reflected radiance (i.e. $V_{terr} = 0$) against the radiance simulated using the two different terrain calculated radiances (from the trigonometric and exact methods). The simulation using the trigonometric approximation was done with the assumption of Lambertian reflection from the adjacent pixels, while in the case of the exact method the anisotropic behavior of the surroundings is taken into account. This will furthermore quantify the impact of non-Lambertian reflection from the neighboring pixels on TOA radiance.

Figure 5.10 shows the RMSD values between the TOA radiance simulations without considering terrain reflected radiance effect versus the simulations applying this effect calculated from the trigonometric approximation (left) and calculated from the exact

method (right). RMSD values are larger for the trigonometric approximation indicating an overestimation of the terrain reflected radiance effect with this approach. On the other hand, the exact method presents very small RMSD over the entire area except the valleys with steep slope. It has been already reported in the literature that this effect is significant for snow covered areas, deep valleys, low sun elevation images and pixels in shadow and can be neglected for other cases due to its intensive computational cost and low impact on the output radiance (Dozier and Frew, 1990; Proy et al., 1989; Richter, 1997). The differences between the two RMSD values in Figure 5.10 can also be related to the assumption on Lambertian reflection from the neighboring pixels, but this assumption seems to have a secondary impact since there is a high correlation between the steep slopes and the RMSD values.

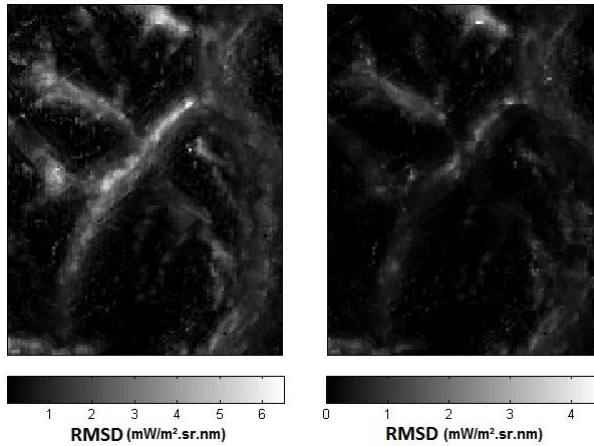


Figure 5.10: RMSD between simulated TOA radiance without applying terrain reflected radiance versus simulated radiance applying terrain reflected radiance calculated with the approximate method (left) and the exact method (right)

The calculation of terrain reflected radiance using the exact method is computationally expensive, since the analysis has to be iterated over all the pixels. In this case study, the computation time for the calculation of the terrain reflected radiance from the exact method was almost 15 hours, while the trigonometric approximation took less than a minute to calculate this effect. This computational cost makes the use of the exact method very limited, in particular it becomes impractical for variable retrieval applications. On the other hand, the trigonometric approximation considers only the slope, which cannot be representative of the amount of the terrain illuminating a given pixel.

We have further carried out an experiment to quantify how significant may be the impact of neglecting topographic effects in terms of variable retrieval. We simulated TOA radiance for different canopy realizations and compared the RMSD between different cases to those found due to topographic effects. This provides an indication as to whether the topographic effects might be neglected without major impacts on retrieval. The TOA radiances (Figure 5.11) were simulated for different cases varying two important canopy variables: LAI and fractional vegetation cover (fCover) for a corn pixel rep-

representative of the study area. Three LAI values, i.e. 2, 2.5 and 3 (m^2/m^2), and three fCover, i.e. 0.58, 0.65 and 0.72 were used for simulations. The values were chosen according to the actual ground measurements of a representative corn pixel in the ESA SEN3EXP field campaign. The leaf chlorophyll content ($40 \mu g/cm^2$), leaf dry matter content ($0.005 g/cm^2$), leaf water thickness (0.019 cm), leaf internal structure variable (1.6) and soil moisture (0.2) were set constant for all simulations (see (Mousivand et al., 2015a) for further details on actual field conditions). The sun zenith angle was 30° and spherical leaf inclination distribution was assumed.

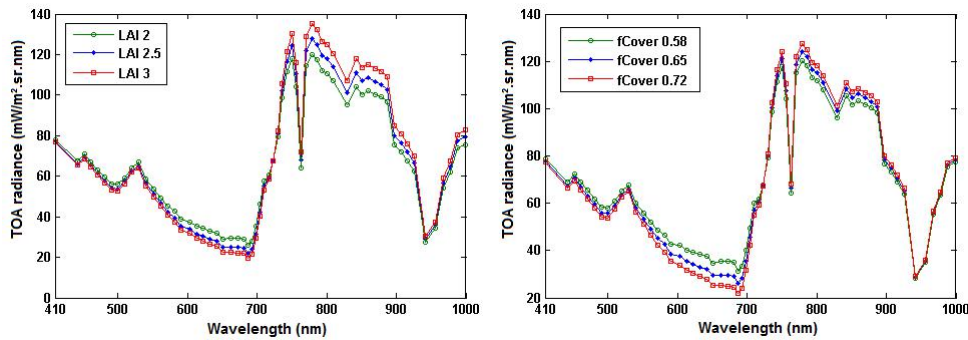


Figure 5.11: TOA CHRIS-Proba radiance simulation using different LAI values (left) and fCover values (right) for a representative corn pixel

The RMSD values between different TOA radiance simulations are given in Table 5.4. A change of 0.5 in LAI results in $RMSD = 4.4$ or $3.9 (mW/m^2.sr.nm)$ depending on the LAI value. A change of 0.07 in fCover also causes the RMSD of 3.2 or 2.7 ($mW/m^2.sr.nm$) depending on the fCover value. The RMSD are significantly higher for larger changes as shown in the table.

Table 5.4: RMSD values between different TOA radiance simulations

Between simulations with	RMSD ($mW/m^2.sr.nm$)
LAI of 2 and LAI of 2.5	4.4
LAI of 2.5 and LAI of 3	3.9
LAI of 2 and LAI of 3	8.2
fCover of 0.58 and fCover of 0.65	3.2
fCover of 0.65 and fCover of 0.72	2.7
fCover of 0.58 and fCover of 0.72	5.9

Referring to Figure 5.9, for example, if the sky view factor is not taken into account over rugged terrain, it would yield an uncertainty up to $5 (mW/m^2.sr.nm)$ in the simulated TOA radiance. Accordingly, we can interpret Table 5.4 as indicating that neglecting this effect can be translated into a change of 0.5 (20% uncertainty) in LAI or similarly 0.07 (10% uncertainty) in fCover in the retrieval of these variables. This means that without considering this effect, provided that all the other effects (atmospheric, radiometric etc)

are considered, an over/underestimation of more than 0.5 in LAI is expected in the retrieval procedure. To understand the importance of the uncertainty caused by neglecting topography effects on the retrieval, it is interesting to know that, for instance, the Global Monitoring for Environment and Security (GMES) user committee has defined an accuracy goal of 10% in the retrieval of vegetation variables to guarantee that the user requirements are met for different applications (Martimort et al., 2007). To this end, topography effects have to be taken into account when retrieving vegetation properties over rugged terrain. The extended four-stream approach presented in this study can be used to account for such effects in the forward simulation of TOA radiance.

5.7. Conclusions

In this study, we aimed at investigating the topographic effect on TOA radiance and variable retrieval by quantifying this effect in terms of considering different topographic components such as sky view factor and terrain reflected radiance. To do so, we presented an extension of “*the four-stream radiative transfer theory*” previously proposed by Verhoef and Bach (2003b, 2007, 2012). The extension is mainly focused on two aspects in TOA radiance modeling. First, the study gives a detailed account of the main topography-induced effects on TOA radiance simulation and the relevant equations are given. Second, a new formulation is proposed for the derivation of the six atmospheric coefficients using MODTRAN in order to make it more computationally efficient, as well as to avoid using zero surface albedo which causes some miscalculations in the results.

To illustrate the topography effects on the TOA radiance, we compared two scenes generated with SLC: the first one for the actual, flat-case, site of Barrax and the second one generated using exactly the same spatial patterns of vegetation properties, but laid over the DEM of a mountain area. Surface reflectance factors were calculated taking into account the impact of topography on the sun-target-sensor geometry. The simulated radiances for shadowed pixels and those exposed to the sun showed considerable differences. It was shown that neglecting sky view factor causes uncertainty in the forward TOA radiance modeling up to 5 ($mW/m^2.sr.nm$) specifically over steep slopes. Two different methods (approximate and horizon methods) were applied to calculate sky view factor and it was concluded that the horizon method delivers better results for forward TOA radiance modeling. The effect of reflected terrain irradiance was also modelled using two different approaches (approximate and exact methods), where the approximate method seems to overestimate this effect. Although the exact method calculates the terrain reflected radiance more accurately, the computational cost of this method limits its use for applications such as variable retrieval. Furthermore, it was shown that, for instance, RMSD of < 5 ($mW/m^2.sr.nm$) due to neglecting topographic effects can cause an over/underestimation of more than 0.5 in LAI (or 0.07 in fCover) in variable retrieval.

This contribution demonstrated that the topographic effect has to be taken into account in variable retrieval. The approach presented here can be used to model TOA radiance over rugged terrain for a range of applications. For instance, retrieving surface properties from a multi-sensor approach using TOA radiance data would require such an approach to accurately simulate the radiance over mountainous areas.

6

Synthesis

6.1. Conclusions

The main objective of this thesis was to improve the retrieval of vegetation properties from optical satellite observations, given the richness of current and near-future sources of optical remote sensing data. This improvement involves different aspects of variable retrieval including model parameterization, forward modeling and inversion algorithm. The primary aim was therefore to gain a better understanding of the key aspects of variable retrieval and to make improvements as regards these aspects. The core hypothesis was that a generic multi-sensor approach designed to integrate a diversity of optical sensors would allow for frequent updates of vegetation biophysical and biochemical variables, as well as it would improve the retrievals compared to any single sensor retrieval. Based on this hypothesis four research questions were defined (Section 1.4). We summarize the answers to the research questions below.

A. Can a sensitivity analysis be exploited to help determining model parameterization and assumptions prior to inversion?

In chapter 3, we addressed this research question. The chapter was designed to investigate how sensitivity analysis can be useful to improve retrieval. Sensitivity analysis quantifies the influence of both individual variables and their interactions on the output radiance (or reflectance). Providing information on the most influential and non-influential variables allows determining which variables are retrievable with the given measurements. Reliable quantitative information can only be retrieved on variables that are closely related to the output radiance. For a given variable, a high sensitivity value indicates significant influence on the output radiance and hence a greater chance of retrieval for that variable. Such a variable can be treated as a free variable during model inversion. On the other hand, a marginal sensitivity value indicates a minor contribution of the variable to the output radiance, which allows setting that variable constant during inversion by assigning it an arbitrary value within its domain.

We assessed the sensitivity of Top-Of-Atmosphere (TOA) radiance and Bottom-Of-Atmosphere (BOA) reflectance to input biophysical and biochemical variables using the coupled SLC-MODTRAN radiative transfer models. The variance-based global sensitivity analysis was applied to different combinations of atmospheric conditions and observation configurations. Four variables including crown coverage (Cv), leaf area index (LAI), leaf inclination distribution function (LIDFa) and soil moisture (SM) were found to be the most influential variables driving the output variance of the radiance from 400 to 2500 nm with a few exceptions among all the inputs. Chlorophyll content (Cab) and water content (Cw) were also identified as influential variables for the visible and short-wave infrared spectral range, respectively. Contrariwise, the dissociation factor, LIDFb and Hapke's soil parameters (h, B0 and c) were found to have marginal influence on the output radiance. The study revealed that the interactions among variables in the the green visible wavelength are responsible for a significant degree of uncertainty in the output radiance, however the red radiance, seems to be less related to the interaction effects. The sensitivity results on TOA radiance were also compared with the results on BOA reflectance. It was concluded that generally TOA radiance sensitivities to dominant biophysical variables are similar to BOA reflectance sensitivities under a clear at-

mosphere (e.g. visibility of 23 km). This is important and suggests that both TOA radiance and BOA reflectance can be applied to retrieve vegetation properties provided TOA data are acquired under good atmospheric conditions.

Since the computational burden of global sensitivity analysis can be considerable, in particular in the case of coupled RT models, we introduced an improvement in the design and sampling of screening methods for efficient sensitivity analysis of computationally expensive models. The improvement was based on a Sobol sampling strategy and winding stairs parameter variation. The results demonstrated that the proposed improvement is efficient in determining influential and non-influential input variables compared to the variance-based method with modest computational demands (only 1200 model runs against 49,152 model runs in the variance-based method). In general, therefore, it seems that the proposed design can be used instead of complex global methods when the goal is to identify influential and non-influential variables among many others, or with computationally expensive methods. Particularly, it is useful where fast and appropriate sensitivity estimates of a coupled surface-atmosphere radiative transfer model at low computational cost is required.

B. Is a generic optical multi-sensor approach using TOA radiometric data to retrieve biophysical and biochemical vegetation variables feasible?

We addressed this research question in chapter 4. A generic multi-temporal, multi-sensor approach was proposed to retrieve biophysical and biochemical vegetation variables using spectral-directional radiometric data. The approach is designed to exploit a temporal sequence constructed by combining data acquired by different sensors over time. The focus was the retrieval of three important vegetation state variables; LAI, fCover and chlorophyll content over the agricultural test site in Barrax, Spain. A variety of different satellite observations including, CHRIS-Proba, Landsat TM and ASTER was used to invert the coupled SLC-MODTRAN4 RT model. Observations and ground truth measurements acquired during the ESA SEN3EXP field campaign were used for model validation.

In the proposed approach, the surface properties are stored in a geo-database and the properties of interest are updated by means of satellite observations. In this sense, retrievals with current observation are incorporated as prior information in the successor observations. When a new observation becomes available, first, the dimensionality of the dataset is explored to determine the possible number of parameters and variables that can be retrieved. Second, the sensitivity analysis is performed to identify the retrievable variables that can be updated in the geo-database given the characteristics of the sensor. Finally, the iterative Bayesian model inversion is employed to invert the coupled RT model versus TOA radiance data.

In the Bayesian model inversion, the observations and a priori knowledge are weighted by their (co)variance matrices. The bit-plane method is used to estimate observation (co)variance matrix, and the posterior covariance matrix of retrievals from one observation is used as prior (co)variance matrix for the successor retrieval procedure. Moreover, depending on temporal auto-correlation between observations (i.e. images), an additional component of variance (i.e. a temporal constraint) was added to the variance of

the prior variables to allow for evolution in time. Differences in the characteristics (spectral, radiometric, spatial and angular) of different sensors results in a number of challenges to implement the multi-sensor approach. We have discussed such challenges in this chapter and corresponding suggestions and solutions are given.

The results showed that integrating information from different sensors improves the retrieval of vegetation structural variables; LAI and fCover. However, the agreement between retrieved and measured values for leaf chlorophyll content was poorer. LAI and fCover were retrieved with RMSE = 0.7 (m^2/m^2) and 0.1 respectively (multiple sensors), while RMSE = 1.09 (m^2/m^2) and 0.15 respectively, when using data acquired by a single sensor. A significant positive correlation was also found between retrievals of LAI and, in particular, fCover (with more than 0.80 for all cases) versus ground measurements in the multi-sensor approach. It was also found that the results were different in terms of crop type. In general, the agreement between measured and retrieved LAI and fCover was better for crops with medium to dense vegetation cover, likely due to better model characterization and situation of such crops that is closer to the model assumption (e.g. the turbid medium assumption used in 4SAIL2). Furthermore, we investigated incorporating prior information from identical sensor type against different sensor types in the multi-sensor approach. In this case, marginal improvement was observed for cases where two identical sensors are combined within a short time period compared with combining different sensors.

The usefulness of the Bayesian model inversion in biophysical variable retrieval was also emphasized. This proposed approach combines the strengths of Bayesian inference and data from a variety of different sensors. The approach can be applied to multispectral and hyperspectral data acquired by different sensors over time. This could be, for instance, applied to different sequences of sensors and data, either current (e.g. Landsat, SPOT, Rapid Eye etc.) or future (e.g. Sentinel 2 and 3).

C. What are the advantages of a multi-sensor variable retrieval over a single sensor variable retrieval approach?

This question was addressed in chapter 4. In this chapter, a comparison between the multi-sensor and single sensor variable retrievals was done. Most available satellite vegetation products rely on measurements from a single sensor. Such retrievals are subject to several inherent limitations. First, the limited number of independent measurements provided by a single sensor, given a large number of variables determining spectral radiance, makes the retrieval problem ill-posed. To overcome the ill-posedness, in most cases the retrieval has to be restricted to only a very few variables (e.g. one or two) and for the other variables fixed values are assumed. Second, the temporal resolution of available optical sensors does not allow for frequent acquisitions. Therefore, due to the revisit time of the sensors and cloud cover, updates of vegetation properties are limited when using data from only one single sensor. Third, single-sensor delivered products over the same area and the same time often show some discrepancies because of the underlying assumptions (e.g. Lambertian soil reflectance, homogeneity of vegetation canopies etc.), as well as the inversion algorithms and forward models used in the retrieval. Such products often come with no measure of uncertainty of the retrieved variables. This makes the comparison of products from different sensors problematic.

The retrievals using data acquired by three different sensors (when only radiometric data are used) were compared to the results with the multi-sensor approach. The multi-temporal, multi-sensor approach was shown to provide time series of vegetation properties by exploiting heterogeneous temporal sequences. In this sense, even when no satellite observations are available due to cloudiness or orbital configuration, the prior retrievals are taken. Furthermore, in almost all cases the accuracy obtained with the multiple sensors retrieval over time was higher than when using a single sensor. This shows that a set of sensor data types with different sensitivities to vegetation properties would lead to more accurate results than those from any single sensor data type. The Bayesian inversion also provided an estimation of the uncertainty of the retrievals. It was concluded that the multi-temporal, multi-sensor approach can contribute to generate a single set of consistent vegetation data products instead of multiple sensor-dependent products, as well as increasing the frequency of usable data on vegetation properties.

D. How significant are the topographic effects on TOA radiance in terms of variable retrieval?

We addressed this research question in chapter 5. Top of canopy reflectance have been frequently used for variable retrieval over the past decades and there exist a number of radiative transfer models to accurately calculate top of canopy reflectance. The potential of TOA radiance for variable retrieval has been also outlined in both this study (chapter 4) and other studies recently (e.g. Laurent et al. (2011a)). TOA radiance modeling requires coupling surface and atmosphere radiative transfer models. The four-stream approach proposed by Verhoef and Bach (2003b, 2007) has been demonstrated to provide reasonably accurate simulations of TOA radiance signature of vegetation canopies (Verhoef and Bach, 2007; Widlowski et al., 2007). We also demonstrated the capability of the four-stream approach to simulate TOA radiance of different sensors over the flat agricultural Barrax area in chapter 4. The approach was initially proposed to simulate TOA radiance of flat vegetated terrains and recently (Verhoef and Bach, 2012) was extended to account for sloped terrains as well. Topography influences the fraction of the incoming direct and diffuse radiation on a surface and modifies the sun-target-sensor geometry, which in turn causes variations in the observed radiance. Retrieval of surface-atmosphere properties from top of atmosphere radiance may need to account for topographic effects. In this chapter, we investigated the topographic effect on TOA radiance and variable retrieval by quantifying this effect in terms of considering different topographic components such as sky view factor and terrain reflected radiance. To account for topographic effects, we proposed an extension of “the four-stream radiative transfer theory” (Verhoef and Bach, 2003b, 2007, 2012) with the focus on representing topography-induced contributions to TOA radiance modeling. A new formulation was also given for the derivation of the six atmospheric coefficients from MODTRAN to make it more computationally efficient. To illustrate the effect of topography on the TOA radiance, we compared two scenes generated with SLC: the first one for the actual, flat-case, site of Barrax and the second one generated using exactly the same spatial patterns of vegetation properties, but laid over the DEM of a mountain area. It was shown that neglecting sky view factor causes uncertainty in the forward TOA radiance modeling up to 5

($mW/m^2.sr.nm$) specifically over steep slopes. The effect of reflected terrain radiance was also modelled using two different approach (approximate and exact methods), where the approximate method seems to overestimate this effect. Although the exact method calculates the terrain reflected radiance more accurately, the computational cost of this method limits its use for applications such as variable retrieval. Furthermore, it was shown that, for instance, RMSD of < 5 ($mW/m^2.sr.nm$) due to neglecting topographic effects can cause an over/underestimation of more than 0.5 in LAI (or 0.07 in fCover) in variable retrieval. Having compared the modeled radiances over the flat- and rugged-case, it was shown that the proposed extension is capable of capturing the topography-induced effects on the modeled TOA radiance over rugged terrains.

6.2. Reflection

The outcomes of this study contribute to improve retrieval of vegetation properties. The first part of this thesis focused on model parameterization for variable retrieval. It was shown that a sensitivity analysis can help in model parameterization. The sensitivity analysis and dimensionality estimation provide a quantitative basis to determine the number and kind of retrievable variables. The number and kind of retrievable variables is crucial in designing a multi-sensor retrieval approach where a variety of different sensors are combined.

The study provides a proof of concept on the retrieval of vegetation properties from multi-sensor spectral-radiometric data. The procedure described and evaluated in this study is designed for the exploitation of a temporal sequence constructed by combining data acquired by different sensors over time. Combining different sensors regardless of their differences allows having more data for a certain area over time and, hence, increases the chance of obtaining frequent updates of vegetation properties. The variable retrieval is carried out using TOA radiance rather than using frequently used top of canopy reflectance data. Performing variable retrieval using TOA radiance has the advantage of avoiding to separate atmospheric correction of image data and retrieval. TOA radiance retrieval also requires no normalization on data from different sensors (e.g. spectral and angular normalization) in a multi-sensor approach. The proposed approach stores the retrieved properties in a geo-database, where they are updated according to the acquired satellite observations. Storing the retrieved properties in a Geographic Information System (GIS) geodatabase makes it possible to benefit from GIS analysis on the retrieved maps.

A further contribution of this study was the number of simultaneously retrieved variables from satellite observations. Most studies have only focused on retrieving a few variables (e.g. one or two) simultaneously. An ideal variable retrieval is one that can retrieve all the influential input variables concurrently. This may seem impractical because of the ill-posedness of the retrieval problem, but the stored maps of surface properties serve as prior information for the successor retrieval and allow better regularization of the retrieval problem to overcome the ill-posedness. The study also showed that the dimensionality of the multi-angular sensors (CHRIS-Proba in this study) was higher than mono-angular sensors. Better regularization along with high dimensionality in a multi-sensor approach allows retrieving more variables simultaneously. For instance, we retrieved six surface biophysical variables using the multi-sensor approach in our case

study. Moreover, the retrieval of some variables such as fraction of brown leaves, LIDF etc. that are not easily retrievable (even measurable) can offer a new direction for variable retrieval. Such variables are the usual candidates to be kept fixed during inversion in most studies. Therefore, a demonstration that such variables can also be retrieved successfully will be a significant step forward in the context of vegetation variable retrieval.

Additionally, this study showed the usefulness of the Bayesian model inversion in biophysical variable retrieval. The Bayesian approach generally implies a subjective view of probabilities in which the prior information quantitatively express degrees of subjective belief in the estimation. The degree of belief in the prior information and the radiometric data is expressed by the observation and prior covariance matrices in the Bayesian model inversion. Therefore, these matrices have to be carefully estimated. We used the sensor NedL as a measure to describe the quality of radiometric data and to fill the diagonal elements in the observation covariance matrix. The bit-plane method was applied to estimate image noise standard deviation. The method is insensitive to spatial texture of the image and preferable to traditional noise estimators requiring the selection of homogeneous areas in the image. The prior covariance matrix was filled with uncertainty values estimated from the predecessor retrievals, stored in the geo-database. Although, we deemed that the estimation of covariance matrices in this way is an appropriate form of weighing different spectral bands, as well as prior information, this aspect requires more consideration for future studies. A further advantage of Bayesian model inversion is that the approximate posterior covariance can be estimated from the curvature of the cost function at its optimal solution. This posterior covariance provides an estimation of the uncertainty of the retrieved variables.

Finally, this thesis contributes to investigate the topographic effect on forward TOA radiance modeling and variable retrieval. It was demonstrated that neglecting topographic effects such as sky view factor or reflected radiance from neighboring slopes can cause notable uncertainty in the forward TOA radiance modeling and hence on the variable retrieval over rugged terrain. The proposed extension of the four-stream TOA radiance modeling approach allows taking into account the topographic effect on TOA radiance. Therefore, the multi-sensor approach presented in this study would also be suitable for use over non-flat areas as well.

6.3. Outlook and future perspectives

This research covered several aspects and contributed to improve our knowledge of physically-based retrieval from satellite observations. Following the research presented in this thesis, efforts should be made in the following domains for future studies.

- The multi-sensor approach presented in this thesis was evaluated over a limited number of remotely sensed data acquired during a short period in the Sentinel-3 Experiment (SEN3EXP 2009) field campaign. Such a short period dataset may not properly represent variability in the time domain for model validation. It is therefore suggested to evaluate further the approach both in terms of time variability and also including more satellite observations. A multi-sensor temporal sequence could be easily constructed with current imaging radiometers such as RapidEye (REIS), SPOT4 (HRVIR1) and Landsat 8 (OLI) images or with near future systems

such as SENTINEL 2, EnMap and PRIMA for future studies.

- The computational time of the multi-sensor approach is still a crucial consideration for operational mapping of vegetation biophysical variables for regional and global applications and has to be reduced considerably. Further research will need to focus on computational complexity issues.
- This thesis carried out the variable retrieval using TOA radiance. More research is still needed to investigate variable retrieval from TOA radiance taking into account different aspects such as adjacency effect and topography effects.
- In this research, the focus was given to the integration of a series of optical image data. Other observation concepts, such as the synergy of a canopy LiDAR and an imaging spectro-radiometer seem a very promising perspective and a scientific challenge for future studies.

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List of Publications

1. **Mousivand, A.**, Verhoef, W., Menenti, M. & Gorte, B. (2015). Modeling Top of Atmosphere radiance over heterogeneous non-Lambertian rugged terrain. *Remote Sensing*, 7(6), 8019-8044.
2. **Mousivand, A.**, Menenti, M., Gorte, B., & Verhoef, W. (2015). Multi-temporal, multi-sensor retrieval of terrestrial vegetation properties from spectral-directional radiometric data. *Remote Sensing of Environment*, 158, 311-330
3. **Mousivand, A.**, Menenti, M., Gorte, B., & Verhoef, W. (2014). Global sensitivity analysis of the spectral radiance of a soil-vegetation system. *Remote Sensing of Environment*, 145, 131-144
4. Villa, P., **Mousivand, A.**, & Bresciani, M. (2014). Aquatic vegetation indices assessment through radiative transfer modeling and linear mixture simulation. *International Journal of Applied Earth Observation and Geoinformation*, 30, 113-127
5. Li, J., Menenti, M., **Mousivand, A.**, & Luthi, S. (2014). Non-Vegetated Playa Morphodynamics Using Multi-Temporal Landsat Imagery in a Semi-Arid Endorheic Basin: Salar de Uyuni, Bolivia. *Remote Sensing*, 6, 10131-10151
6. Jokar arsanjani, Jamal, Marco Helbich, & **Mousivand, A.**. A morphological approach to predicting urban expansion. *Transactions in GIS* 18.2 (2014): 219-233.
7. Jokar arsanjani, Jamal, Wolfgang Kainz, & **Mousivand, A.**. Tracking dynamic land-use change using spatially explicit Markov Chain based on cellular automata: the case of Tehran. *International Journal of Image and Data Fusion* 2.4 (2011): 329-345.