

COMPOSITION DU JURY

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LIST OF ABBREVIATIONS

ANN: Artificial Neural Networks
APEX: Airborn Prism Experiment
ASD: Analytical Spectral Device
BAI: Broadband Spectral Angle Index
BSI: Bare Soil Index
C: Carbon
CAI: Cellulose Absorption Index
CB: Cubist Algorithm
CDPC: Central Data Processing Center
CF: Carbon Farming
CNN: Convolutional Neural Networks
CRA-W: Walloon Agricultural Research Center
CV: Coefficient of Variation
DLR: German Aerospace Centrum
DSM: Digital Soil Mapping
EU: European Union
GBT: Gradient Boosting Trees
GEE: Google Earth Engine
GHG: Greenhouse Gas
GPS: Global Positioning System
HYSOMA: HYperspectral SOil MAPper
IEEE: Institute of Electrical and Electronics Engineers
K: Potassium

List of Abbreviations

LPL: Lower Prediction Limit

LUCAS: Land Use/cover Area frame Survey

LULUCF: Land Use, Land Use Change and Forestry

LV: latent variable

MAJA: Multi-Mission Atmospheric Correction and Cloud Screening software – Atmospheric Correction Joint Algorithm

MDD: Minimum Detectable Difference

MEC: Model Efficiency Coefficient

MIR: Mid-Infrared

MLR: Multiple Linear Regression

MRV: Measurement, Reporting and Verification

MSE: Mean Squared Error

MSI: Multispectral Instrument

N: Nitrogen

NBR2: Normalized Burn Ratio

nCAI: normalized Cellulose Absorption Index

NDVI: Normalized Difference Vegetation Index

NIR: Near-Infrared

NPP: Net Primary Production

NSMI: Normalized Soil Moisture Index

OC: Organic Carbon

OLS: Ordinary Least Squares

OM: Organic Matter

P: Phosphorus

PCR: Principal Component Regression

List of Abbreviations

PIR:	Prediction Interval Range
PLSR:	Partial Least Squares Regression
POC:	Particulate Organic Carbon
RMI:	Royal Meteorological Institute
RMSE:	Root Mean Square Error
RPD:	Ratio of Performance to Deviation
RF:	Random Forest
RGB:	Red-Green-Blue
RT:	Regression Trees
RTK:	Real Time Kinematic
SAR:	Synthetic-Aperture Radar
SD:	Standard Deviations
SDG:	Sustainable Development Goal
SE:	Standard Error
SNR:	Signal-to-Noise Ratio
SOC:	Soil Organic Carbon
SOM:	Soil Organic Matter
SVMR:	Support Vector Machine Regression
SWIR:	Short-Wave-Infrared
S-1:	Sentinel-1
S-2:	Sentinel-2
S2WI:	Volumetric Soil Moisture
UAV:	Unmanned Aerial Vehicle
UNFCCC:	United Nations Framework Convention on Climate Change

List of Abbreviations

UPL: Upper Prediction Limit

UV: Ultraviolet

VIP: Variance Importance Projection

Vis: Visible

WISOIL: Water Index Soil

LIST OF PUBLICATIONS

Parts of this thesis (3 chapters) have been published in peer-reviewed journals:

[1] Dvorakova K., Shi P., Limbourg Q. & van Wesemael Bas. (2020) Soil organic carbon mapping from remote sensing: the effects of crop residues. **Remote Sensing**, 12, 1913-1938. doi:10.3390/rs12121913

[2] Dvorakova K., Heiden U. & van Wesemael B. (2021) Sentinel-2 exposed soil composite for soil organic carbon prediction. **Remote Sensing**, 13, 1791-1812. doi.org/10.3390/rs13091791

[3] Dvorakova K., Heiden U., Pepers K., Staats G., van Os G. & van Wesemael B. (2022) Improving soil organic carbon predictions from a Sentinel-2 composite by assessing surface conditions and uncertainties. **Geoderma**, 116128

CHAPTER 1. INTRODUCTION

1.1 GENERAL INTRODUCTION

Human activities have gradually influenced the carbon (C) cycle by redistributing massive amounts of carbon from the geosphere and pedosphere into the atmosphere, thus causing a climate change (Riebeek 2011). Soils form the largest pool of terrestrial organic carbon (1500 Pg C in the first meter of soil, (Le Quéré et al. 2014)). Sanderman et al. (2018) have estimated that centuries of cropping have resulted in the transfer of 133 Pg C from the soil to the atmosphere. Therefore, the concern about the role of soils in the global carbon budget and the effects of soil organic carbon (SOC) decline on soil quality has been incorporated into international treaties.

The United Nations Framework Convention on Climate Change (UNFCCC) have set up the Paris Agreement in 2015, whose aim is to keep the rise in mean global temperatures to well below 2°C above pre-industrial levels (UNFCCC 2021). In conjunction with the UNFCCC Paris Agreement, the French government has proposed the '4 per mille Soils for Food Security and Climate' international initiative. Its aim is to increase soil C in a large portion of agricultural soils globally, by 0.4% per year. This would produce a C sink increase of 1.2 Pg C per year, hence slowing down climate change (Minasny et al. 2017). Another two examples of soil C sequestration strategies are conservation agriculture (CA), and carbon farming (CF), where farmers apply management practices that help restore carbon in the soil.

Implementation of such initiatives requires a robust, scientifically-sound measurement, reporting and verification (MRV) system to track that the policy goals are being met and that claimed increases in soil C stocks in croplands are

real (Paustian et al. 2019). Consequently, many studies focus on the spatio-temporal SOC dynamics.

Remote sensing offers the possibility of providing indirect information on soil data (McBratney et al. 2003). Combined with field observations (i.e. soil samples), remote sensing gathers an important amount of data in a cost- and time-effective way. However, the process of deriving final soil product from remote sensing imagery is hindered by a number of factors, such as the condition of the soil surface, which needs to be bare.

1.2 PROBLEM STATEMENT

As part of an efficient soil monitoring system, there is need for cost-effective and accurate SOC maps of croplands that cover large areas (regional/national), with high spatial (~20-50m) and temporal (five years repeatability) resolution. Conventional soil mapping (e.g. kriging) methods are currently considered to be ineffective for high resolution monitoring at a reasonable cost and time (Zeraatpisheh et al. 2017). Digital soil mapping (DSM), on the other hand, is a powerful technique which is increasingly applied by soil scientists to map soil properties using ancillary data, among which remote sensing products (McBratney et al. 2003). Kempen et al. (2012) and Andries et al. (2021) performed a cost-accuracy analysis of the various SOC mapping approaches, and found that the cost of digital soil mapping could be reduced by a factor of three compared with conventional approaches, without compromising accuracy. This cost reduction is mainly linked to a lower sampling density required for digital soil mapping, as traditional methods based on soil sampling and laboratory analysis are expensive and time-consuming (Andries et al. 2021). The lower density of samples is compensated by the large stream of information originating from remote sensing products. Therefore, **the potential of remote sensing products to provide rapid, repeatable, cost-effective**

and accurate monitoring systems for SOC is of considerable interest.

Multiple studies (Castaldi et al. 2019a; Castaldi et al. 2018; Castaldi et al. 2019c; Chabrilat et al. 2019; Gholizadeh et al. 2018; Guo et al. 2019; Moura-Bueno et al. 2019; Vaudour et al. 2016; Vaudour et al. 2019a) have demonstrated the suitability of remote sensing techniques for SOC mapping in croplands, given their large spatial coverage and high temporal resolution. It has however been shown that **the assessment of SOC may be hampered by the disturbing effects of crop residues, moisture, vegetation and roughness at the soil surface.** Therefore, **conditions under which spectral models can be developed and applied to produce reliable SOC prediction maps must be clearly defined.** Moreover, a survey amongst experts in soil health and policy areas performed by Andries et al. (2021) has shown that **validation accuracy of 90% would be required from SOC mapping techniques to be acceptable as part of an effective monitoring system.**

1.3 OBJECTIVES OF THE THESIS

The overall aim of this thesis is to minimize or remove most of the issues that have a negative effect on the SOC prediction accuracy from remote sensing. This will potentially improve the SOC maps, making them suitable for operational use.

The specific objectives of this research are to:

- 1. assess the effects of disturbing factors on SOC prediction from Sentinel-2 and removing/correcting them**

Using the combination of airborne hyperspectral imagery and Sentinel-2 (S-2) spaceborne multispectral imagery on a pilot zone, we firstly focus on finding a spectral index that allows to eliminate pixels affected by crop residues. Once

this index is found, we proceed to create an automated method using S-2 time series which allows to select soil pixels in suitable conditions (i.e. dry, bare and freshly ploughed), based on the cropping period.

2. create Sentinel-2 exposed soil composites for SOC mapping in Wallonia

This second objective allows to apply the knowledge found in the first objective at a larger scale, i.e. Wallonia. We begin by creating exposed soil composite using Google Earth Engine processor, and we use it to create a SOC map. Additionally, the uncertainty and the accuracy of the SOC map is assessed.

3. test the potential of the created SOC maps as a tool for detecting areas under conservation agriculture and carbon farming

Using as input the SOC map created in the second objective, we test whether fields undergoing conservation agriculture and carbon farming practices show higher SOC contents, compared to fields under conventional agriculture.

1.4 OUTLINE OF THE THESIS

This thesis is based on articles published or submitted to international peer-reviewed journals.

Chapter 2 offers an overview of the literature that exists on the topic of SOC, from its underlying importance for good soil functioning, to the various methods of measuring SOC by spectroscopy techniques. A brief introduction of the study area and the material used end the second chapter.

Airborne hyperspectral image of a pilot zone in Wallonia is used to assess the effect of crop residues on SOC prediction models in Chapter 3. A hyperspectral index, Cellulose Absorption Index (CAI), is used to this end. Additionally, we scale up to spaceborne multispectral

imagery (S-2) and attempt to find a multispectral index that is capable of detecting crop residues on soil surface.

Chapter 4 focuses on developing an automated method for bare soil detection. We hypothesize that there is a window in the cropping calendar, during which the surface conditions reflect the spectral signature of the soil. This occurs when soils are dry and in seedbed condition, and therefore are harrowed and without any green vegetation or crop residues. Using S-2 time series, we create a methodology that allows detecting the appropriate window of suitable soil surface conditions.

In Chapter 5 we define, an appropriate methodology for creating suitable exposed soil composites for SOC mapping from S-2. For this, in-situ field observations of the soil surface conditions of croplands in Belgium are acquired, and are linked to their spectral signature extracted from S-2 imagery. These observations allow to determine spectral index thresholds which will be used to obtain soil composite including only pure soil spectra. This composite is then used to create SOC prediction maps. Additionally, the uncertainty of prediction of these maps is assessed.

Chapter 6 tests the potential of the SOC maps to detect the effect of carbon farming and conservation agriculture on topsoil SOC content. Two datasets containing fields undergoing conservation agriculture practices and carbon farming practices were collected. We use a matching technique to select fields under conventional agriculture, where we control for the pedologic and climatic variables that play a role in the SOC sequestration potential. Comparing the predicted SOC in the original datasets with their matched datasets, we evaluate what effect the various management practices have on the SOC content

The general conclusion in Chapter 7 provides an overview of the main findings and the limitations encountered. The perspectives are given in order to motivate further research.

CHAPTER 2. LITERATURE REVIEW

OUTLINE

It is generally recognized that soils form the largest pool of terrestrial organic carbon. Therefore, even small changes in SOC stocks have a large impact on CO₂ concentrations in the atmosphere. Consequently, it is of foremost importance to detect low/high SOC environments in order to improve soil management and limit negative impacts of human activities on global warming and soil degradation. This chapter provides a brief outline of institutional context. Firstly, the role of soils in the global carbon cycle is uncovered. Secondly, the SOC and its defining factors are discussed. Thirdly, we present the existing SOC modelling techniques using remote sensing imagery and their applications. A brief introduction of the study area and the material used end this second chapter.

2.1 PARIS AGREEMENT

An international treaty on climate change was signed in 2015 under The United Nations Framework Convention on Climate Change (UNFCCC). This treaty, the Paris Agreement, aims to keep the rise in mean global temperature to well below 2°C above pre-industrial levels, and preferably limit the increase to 1.5°C, to substantially reduce the effects of climate change (UNFCCC 2021). To reach this goal, emissions need to be cut by 50% by 2030. 193 country members of the UNFCCC have ratified the Paris Agreement, including all member states of the European Union (EU) (UNFCCC 2021). As part of achieving the goals of the Paris Agreement, countries, regions and companies are establishing zero-carbon solutions, which

have become competitive across economic sectors representing 25% of emissions worldwide. The trend is most noticeable in the power and transport sectors (UNFCCC 2021). The Land Use, Land Use Change and Forestry (LULUCF) sector has been gaining interest as a sector with high potential for achieving the goal of climate neutrality (COWI 2021). It is generally recognized that soils form the largest pool of terrestrial organic carbon (OC). The soil organic carbon (SOC) pool has been estimated to contain 1500 Pg C in the first meter of soil, which is more OC than both biosphere (roughly 500 Pg C) and atmosphere (roughly 800 Pg C) combined (Le Quéré et al. 2014; Stockmann et al. 2015). Therefore, SOC contained in all biotopes is considered a major pool in the global C-cycle, and losses or gains of SOC have a large impact on CO₂ concentrations in the atmosphere (Le Quéré et al. 2014).

2.1.1 Agricultural soils as carbon sink or carbon source

About 45% of global soils are under some form of agricultural use (i.e. cropland and grazing land) (Paustian et al. 2019). The vast majority of agricultural lands are on mineral soils, i.e. soils where OC makes up a small fraction (~1-5%) of the total soil mass which is dominated by mineral matter (i.e. sand, silt and clay particles) (Paustian et al. 2019). Most agricultural soils are depleted in C relative to the native ecosystems from which they were derived (Paustian et al. 2019). According to Davidson and Ackerman (1993), most cropland mineral soils have lost 30–50% of the C stocks in top soil layers (0–30 cm) relative to their native condition. Sanderman et al. (2018) have estimated that centuries of cropping have resulted in the loss of 133 Pg C from the soil. In 2015, agricultural production contributed 10-14% of the total greenhouse gas (GHG) emissions. Therefore, there is a strong motivation for the inclusion of soil-centric mitigation projects that turn

agricultural soils into carbon sink, to reach the Paris Agreement goal of 2030.

2.1.2 Soil carbon sequestration initiatives

The OC content of soils is governed by the balance between the rate of C added to the soil from plant residues and organic amendments (e.g., manure, compost), and the rate of C lost from the soils, which is mainly as CO₂ from decomposition processes (Paustian et al. 2019). Soil C sequestration strategies rely on management practices that increase the amount of carbon stored as soil organic carbon (Paustian et al. 2016). They could be applied at large scales and potentially at low costs. For example, in conjunction with the UNFCCC Paris Agreement, the French government has proposed the '4 per mille Soils for Food Security and Climate' international initiative. Its aim is to increase soil C content in a large portion of agricultural soils globally, by 0.4% per year. This would produce a C sink increase of 1.2 Pg C per year (Minasny et al. 2017).

Recently, the EU has proposed a legislative framework for sustainable agriculture, called The Farm to Fork Strategy (2019). This strategy aims to accelerate the transition to a sustainable food system by helping to mitigate climate change and ensure food security (COWI 2021). One of the pivot points of The Farm to Fork Strategy is Carbon Farming (CF). In CF, farmers are offered incentives to improve their farming practices and safeguard the environment, through the application of mitigation actions at farm level to manage carbon and GHG fluxes.

Implementation of such policies however requires robust, scientifically-sound measurement, reporting, and verification (MRV) systems to track that policy goals are being met and that claimed increases in soil C stocks are real (Paustian et al. 2019). Such MRV system should have high temporal repeatability, and require limited ground-

based data to be cost-effective. The use of remote sensing can help to obtain such MRV system (Paustian et al. 2019). However, so far, it is the accuracy and the verifiability of the MRV systems that is the limiting factor hindering the implementation of soil C sequestration policies.

2.2 SOIL ORGANIC MATTER, SOIL ORGANIC CARBON AND SOC STOCKS

Net Primary Production (NPP) is the net flux of carbon from the atmosphere to vegetation per unit of time. The annual gain of energy and matter by the vegetation is distributed within any terrestrial ecosystem in three ways (Swift et al. 1979): (i) a variable portion of the NPP contributes to the net growth of the plant system, (ii) a small part is consumed by herbivores and (iii) the rest enters the decomposition process mainly in the soil where micro-organisms (bacteria and fungi) and invertebrates use dead organic matter (plant and animal residues) as energy and nutrient supply for their own growth. All organic components in the soil, excluding the undecayed plant and animal tissues, form the soil organic matter (SOM). Elsevier's Dictionary of Soil Science (Canarache et al. 2006) defines SOM as «[...] the totality of organic components of the soil solid phase, consisting of both non-humic substances [part of SOM made up of undecomposed or partially decomposed organic materials (mainly carbohydrates and peptides) (Watanabe and Kuwatsuka 1993)] and humus [humic substances synthesized from decomposed plant and animal residues]. » (p. 807). SOM is used in the assessment of soil quality and agricultural productivity due to its influence on soil physical, chemical and biological properties. It is critical for its (1) soil structure stabilization, (2) retention and release of plant nutrients, (3) water-holding capacity and (4) cation exchange capacity (Lal and Bruce 1999).

Soil organic carbon (SOC) is defined in Elsevier's Dictionary of Soil Science (Canarache et al. 2006) as « [...] the C found

in the soil organic matter. It includes remnants of plants, animals, and micro-organisms in all stages of decomposition, as well as humus [...] » (p. 807). SOC is estimated to amount on average to 58 percent of SOM by mass (Nelson and Sommers 1983). Usually, it is SOC that is analyzed in soil samples, and it is therefore used as proxy for SOM.

SOC content [g C kg^{-1}] is defined as the mass of OC (in g) contained in one kg of soil (Equation 2.1):

$$OM = 1.72 \times SOC_{cont} \quad (\text{Equation 2.1})$$

where OM [g C kg^{-1}] is the content of SOM. This conversion factor is defined in agricultural soils based on the assumption that OM contains 58% OC, but can vary in different soils. A consideration of the possible variation in organic matter composition predicts a range of factor values between 1.4 and 2.5 (Pribyl 2010).

SOC stock [Mg C ha^{-1}] is conventionally defined as the amount of OC in a predefined soil depth (Equation 2.2):

$$SOC_{stock} = \frac{1}{100} \times BD \times SOC_{cont} \times D \times (1 - RM) \quad (\text{Equation 2.2})$$

where D is sampling depth considered [m], BD is the soil bulk density [kg m^{-3}] and RM is the mass proportion of rock fragment content (dimensionless).

The process of transferring CO_2 from atmosphere into the soil, through plants, plant residues and other organic solids which are stored or retained in the soil as part of the SOM, is called *carbon sequestration* (Chenu et al. 2019). It is quantified for a given duration, because retention time of sequestered carbon in the soil can range from short-term (no immediate release back to atmosphere) to long-term (millennia) storage (Chenu et al. 2019). The term *carbon storage*, which is often mistakenly used interchangeably

with *carbon sequestration* is broader. *Carbon storage* is defined as the increase in SOC stocks over time in the soils, not necessarily associated with a net removal of CO₂ from the atmosphere (Chenu et al. 2019).

2.2.1 Factors affecting SOC

The rate at which SOC increases or decreases is controlled by the balance between biomass (mainly from plants) input into the soil (renewal) and the losses through decomposition (removal) (Lal and Bruce 1999). Firstly, atmospheric CO₂ is fixed by plants via photosynthesis whereby C and water are the main building blocks for plant biomass. Secondly, the plant biomass is transferred to the soil, where it may be readily decomposed by microorganisms and is emitted back into the atmosphere as CO₂ and water, or to a lesser extent removed by erosion and leaching as dissolved organic carbon (Lal and Bruce 1999). Overall, SOC stock accrual is a result of (1) an increase in OC inputs, (2) a reduction of C outputs, or (3) a combination of both. An increase can occur through increasing biomass inputs from vegetation (increase in net primary production or in residue return) or through increasing exogenous OM appliance (e.g. manure) (Chenu et al. 2019). A reduction of C outputs can be obtained by reducing mineralization by micro-organisms or SOC erosion (Chenu et al. 2019).

Newly added C can be stabilized in the soil by three mechanisms preventing or hindering decomposition by soil fauna (Six et al. 2002): (i) Physically: formation of stable micro- and macro aggregates renders C inaccessible to microbial decomposition. (ii) Chemically: strong formation of chemical bonds between C and clays prevents consumption by organisms. (iii) Biochemically: re-synthetization of C into complex molecule structures makes SOC non-decomposable by most organisms.

The removal rate is therefore dependent on these mechanisms, which are in their turn affected by land use and management practices, as is the magnitude of C production (Lal and Bruce 1999). Overall, the SOC pool is a dynamic system strongly dependent on many external factors, resulting in a large spatial variation. Spatial variability of SOC can and should be assessed at various scales, as with increasing extent (from field to regional, continental and global scales) an equally increasing spatial variation in SOC occurs (Minasny et al. 2017). Moreover, the vertical SOC gradient also presents significant variations.

2.2.2 Vertical variability of SOC

Numerous studies have focused on the SOC stock of the topsoil (the upper 15 to 30 cm), however it has been established that the upper 0.2 m of soil only contains approximately 40% of the total C in the upper meter (Baisden and Parfitt 2007). Despite the large SOC stock in the deeper soil layers, the C dynamics and factors responsible for vertical distribution of SOC are poorly understood (Meersmans et al. 2009a).

Baisden and Parfitt (2007) reported more stable C with greater turnover times in the deeper soil layers based on radiocarbon ^{14}C dating. Jobbágy and Jackson (2000) showed that C content reaches greater depths than the roots. This suggests decreased decomposition rates of SOC with depth, due to a lack of fresh OC in those deeper layers, which diminishes the energy supply to microbes responsible for decomposition (Jobbágy and Jackson 2000; Lal and Bruce 1999). Leaching and vertical mixing by soil organisms is also thought to be linked to SOC migration into deeper layers, partly explaining the relatively large amounts of C at these depths, however their role is thought to be minor (Jobbágy and Jackson 2000).

Meersmans et al. (2009b) studied the depth distribution of SOC under cropland, grassland and forest with contrasting soil texture and drainage types using an empirical modelling approach. Their findings suggest a similar vertical SOC distribution within soils with similar characteristics. Overall, SOC content showed an exponential decline with depth for all land use, drainage and particle size classes.

2.2.3 Spatial variability of SOC

SOC variability is scale-dependent, because soil properties are influenced by driving factors acting at different levels. At the global scale, SOC spatial variability is driven mainly by climate. SOC stocks in the topsoil (0-0.3m) range from 10 Mg C ha⁻¹ to 160 Mg C ha⁻¹ resulting in global estimates of the total OC pool to 1 m depth between 1463 and 2011 Pg C (Stockmann et al. 2015). Greater SOC stocks occur at higher latitudes, where low temperature regimes and wet conditions decrease biological activity, which in turn lowers the rates of decomposition. SOC stock then decreases in the mid-latitudes and increases again in the humid tropics, where high precipitation and net primary production encourage the input of OC into the soils (Minasny et al. 2017).

At the scale of a nation or of a landscape, SOC patterns become much more erratic, and are mainly controlled by vegetation type, topography (elevation closely associated with temperature and precipitation), land use and soil type (Lal and Bruce 1999; Xin et al. 2016). For instance, herbaceous vegetation with relatively high root biomass produces residues directly into the soil, compared to forested areas, where most OM is produced aboveground and is more resistant to microbial decomposition (Oueslati et al. 2013). Topography directly affects the water movements in soils, resulting in moister soils in depressions and better drained soils in uphill areas. Depressions therefore receive more runoff, which transports sediments

including OM originating in the uphill areas, where OM is lost (Oueslati et al. 2013). With increasing altitude precipitation increases and temperature decreases, which is in favor of greater accumulations of SOC (Xin et al. 2016). Overall, the soil type and texture are controlled by lithology, climate and topographical variables. The lithology defines the soil constituent material, while the latter two in turn affect the hydrology, as stated above, and therefore the SOC stocks (Zhang et al. 2012).

At short range, e.g. a radius of few hundred meters, the variations of SOC may reach the same order of magnitude as the variations over an entire region (Goidts et al. 2009). For instance, images from airborne spectroscopy (e.g. Stevens et al. (2010)) reveal notable differences in SOC content within a single field, as well as between several contiguous fields. Stevens et al. (2015) pointed out a clear distinction between processes that vary within a field and those that vary between fields: for instance, water and tillage erosion and topography related moisture and temperature conditions have an influence on SOC stock that varies within a field, whereas agricultural management and landscape history has a constant effect on SOC within one field.

2.2.3.1 Topography

Topography plays a dominant role in the spatial distribution of hydrological processes, the latter being closely correlated with vegetation growth, displacement processes and decomposition of SOC. Water erosion coupled with hydrological factors that play a role for SOC dynamics promotes conservation of buried C in valley bottoms, where saturation leads to anaerobic conditions with reduced microbial decomposition (Wang et al. 2000).

2.2.3.2 Soil properties

There is a broad consensus that soil texture (i.e. proportion of clay ($<2\mu\text{m}$), silt ($2\mu\text{m} - 50\mu\text{m}$) and sand ($50\mu\text{m} - 2\text{mm}$))

is strongly associated with SOC storage (Wiesmeier et al. 2019). The physical protection of SOM by organo-mineral complexes is an important mechanism for C stabilization (Wiesmeier et al. 2019). The protective capacity of aggregates is related to (1) a spatial separation of substrate and microorganisms, (2) as well as to a reduced microbial activity due to a reduced diffusion of oxygen into aggregates (Wiesmeier et al. 2019). For example, clay-rich soils have been shown to store more SOC than any other soil texture, explained by the association of OM with clay particles resulting in physical and chemical protection of SOC from decomposition (Davidson 1995).

Characterization of SOC chemical composition in different soil size fractions shows that different-sized minerals potentially protect different types of SOC (Han et al. 2016). The much lower mineralization of mineral-associated OC relative to free OC has been frequently reported in the literature, highlighting the potential importance of minerals on the stability of OC in soil (Han et al. 2016). These fractions (smaller than 20µm) are related to stable organic matter and reflect long-term (10-100 years) C storage (van Wesemael et al. 2019). The fraction larger than 20 µm is more heterogeneous, consisting of micro aggregates, small macro aggregate, OM associated with coarse silt and sand, and particulate organic matter (POM) (van Wesemael et al. 2019).

Additionally, soil texture and drainage are intimately linked, as finely-textured soils have smaller pores and therefore a greater ability to retain water, due to capillary forces. The result is generally a poorly drained soil when the particle size decreases, and a well-drained soil with increasing particle size. Many studies (e.g. Davidson (1995); Doetterl et al. (2013); Meersmans et al. (2008)) found a positive correlation between soil wetness and SOC, which suggests that soil drainage has a negative effect on the SOC stock. This is thought to be due to O₂ limitations of decomposition in wet soils (Wang et al. 2000).

2.2.3.3 Management practices

Management practices influence SOC stocks by either increasing C inputs to soil or decreasing SOC losses (Chenu et al. 2019). Many types of practices exist, and they can vary in terms of tillage, organic amendments, fertilizer applications, mulch application, etc. (Chenu et al. 2019). Here, we list a few examples of management practices and their effect on SOC stocks.

Agricultural management systems with crop rotations generally reveal higher amounts of SOC than monoculture systems, driven by enhanced root C input, soil microbial diversity and soil aggregate stability (Wiesmeier et al. 2019). Moreover, crop systems that are dominated by plants with deep root systems promote SOC storage, as retention of root derived C in soil has been found to be 2.3 times higher than for aboveground residues (Wiesmeier et al. 2019).

Tillage is generally considered to increase SOC mineralization due to the mechanical disruption of soil aggregates and the consequent release of CO₂ (Chenu et al. 2019). Therefore no-tillage has been considered as a suitable practice to increase/maintain SOC stocks compared to the conventional tillage (Chenu et al. 2019). However, there is evidence that reduced or no-tillage does not affect SOC storage but only leads to redistribution of SOC within the soil profile (Chenu et al. 2019; Wiesmeier et al. 2019).

Addition of fertilizers and manures has been shown to influence SOC content of croplands (Haynes and Naidu 1998). The application of organic manures results in increased SOC stock, which in turn results in increased water holding capacity, porosity, infiltration capacity and decreased bulk density and surface crusting, and an overall increase in soil quality (Haynes and Naidu 1998). The most common form of chemical fertilization is the application of N, P and K which have been shown to increase the SOC stock, if adequately applied, i.e. respecting the healthy NPK

soil ratio (Galantini and Rosell 2006; Halvorson et al. 1999). Given the current context of global climate change however, it has been stated that a reduction of the use of mineral N fertilizers might be necessary to reduce the associated GHG emissions, as (1) the industrial production of N fertilizers is highly energy consuming and GHG emitting process and (2) nitrification reaction in soils emits large quantities of N₂O (Pellerin et al. 2017).

2.3 MODELLING OF SPATIAL VARIABILITY IN SOC

The previous section listed few examples of the driving factors affecting SOC spatial variability in croplands. Hence, SOC spatial variability results from a complex combination of these factors (McBratney et al. 2003). One can therefore infer that modelling SOC content or SOC stocks is far from evident.

SOC spatial variability can be quantified and modelled by means of multivariate statistics and geostatistics (McBratney et al. 2000). Such models are usually constrained by relatively expensive fieldwork and subsequent laboratory analysis (McBratney et al. 2003). As was already pleaded by Grunwald (2010), the development of cost-effective methods for the collection of soil data is a priority in contemporary soil science. This is particularly important when considering the creation of inexpensive, reliable and fair soil monitoring systems for soil C sequestration policies (section 2.1.2). Fast and cheap sampling techniques are required to offer a large scale system with high temporal resolution, to detect changes in SOC.

2.3.1 Diffuse reflectance spectroscopy

Remote sensing offers the possibility of providing indirect information on soil data (McBratney et al. 2003). Combined with field observations (i.e. soil samples), remote sensing

gathers an important amount of data in a cost- and time-effective way. It is based on the process of diffuse reflectance spectroscopy, where physical properties of an object are determined by measuring its reflected and emitted radiation at a distance (USGS 2020).

Diffuse reflectance spectroscopy relies on the analysis of spectral reflectance, which is itself a function of wavelengths. Reflectance is the percentage of incident light that is reflected from a surface. Every substance possesses its own characteristic spectrum (i.e. the 'fingerprint'), and can be identified by the nature of the reflectance spectrum it provides (Chabrillat et al. 2019). The more wavelengths involved in the measurement scheme, the more information can be obtained about the composition of the object in question (Chabrillat et al. 2019). The form of the spectrum depends on the selective absorption features of chemical constituents and overall shape of the physical properties (Chabrillat et al. 2019). The electromagnetic spectrum is classified in remote sensing literature into five spectral regions (Table 2.1).

Table 2.1: *Regions of the electromagnetic spectrum. After Stevens (2008).*

Wavelength	Region	Abbreviation
250 nm	Ultraviolet	UV
400 nm		
700 nm	Visible	Vis
1.1 μm	Near-Infrared	NIR
2.5 μm	Short-Wave-Infrared	SWIR
25 μm	Mid-Infrared	MIR

2.3.2 Soil spectrum

Soil moisture, organic matter, carbonates, mineralogy, and texture are the main constituents influencing the shape of soil reflectance on the electromagnetic spectrum. Visible (Vis), near-infrared (NIR) and short-wave-infrared (SWIR) regions of the electromagnetic spectrum contain spectral information of soils that shows the highest absolute correlation with OM (Ben-Dor et al. 1997; Viscarra Rossel et al. 2006). Generally, higher SOC content in soils is reflected in darker color. The strong correlation in the Vis region is thought to be due to the direct relation between the darkness of the soil and the OM quantity (Ben-Dor et al. 1997). The optical activity of chemical chromophores (i.e. the parts of a molecule responsible for its color) is due to vibration overtones and combination modes of functional groups at the molecular level across the SWIR spectral region and to electronic transitions in atoms across the Vis-NIR spectral regions (Ben-Dor et al. 1997; Stenberg et al. 2010). More important features are found in the SWIR region, where spectral response varies with specific chemical bonds, such as C-H at 1340-1380 nm or N-H at 1860-1900 nm (Ben-Dor et al. 1997). Moreover, other features like lignin, cellulose and starch, i.e. the main organic compounds, affect the reflectance at 1600-1800 nm, 2100 nm and 2300 nm respectively (Ben-Dor et al. 1997). Tables of absorption positions and their related soil components are published in Ben-Dor et al. (2002), Viscarra Rossel and Behrens (2010) and Soriano-Disla et al. (2014).

Two typical soil spectra with different SOC contents are given in Figure 2.1. As mentioned above, soil reflectance is higher for sample with lower SOC content. Water absorption bands can be observed at 1.4 μm and 1.9 μm .

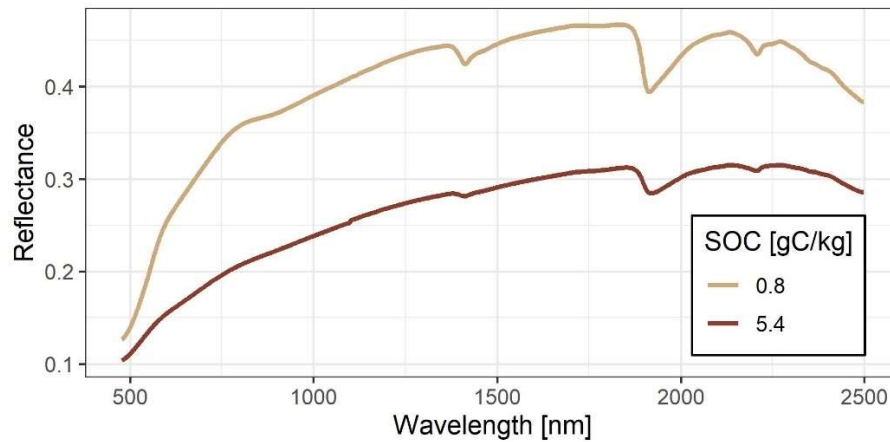


Figure 2.1: *Example of two soil spectra of sandy-loam soils with various SOC contents measured by a laboratory spectrometer.*

2.3.3 Types of spectroscopy

The need for a large amount of spatial data for SOC modelling or prediction favored the appearance in reflectance spectroscopy of new portable solutions (Stevens 2008). Applications at three scale levels can be distinguished: (1) laboratory spectroscopy, (2) field spectroscopy and (3) imaging spectroscopy. In laboratory spectroscopy, spectra are collected one point at a time under controlled environmental conditions. In field spectroscopy, spectra are usually collected one point at a time, but environmental conditions cannot be controlled. Imaging spectroscopy collects data as a two-dimensional array of measurements with a sensor that is usually mounted on a plane, an unmanned aerial vehicle (UAV) or satellite. This means that the quality of the spectral measurements depends on environmental conditions in all cases.

While in principle any object reflects light in the same proportion, independently of the light source or its environment, some factors do disturb the measurement (Stevens 2008). Atmospheric absorption and scattering,

surface scattering, illumination geometry, shadowing, internal characteristics of the instrument or user manipulation affect the measurements in such a way that the reflectance recorded by any sensor differs from the real spectrum.

2.3.3.1 Proximal spectroscopy

Laboratory spectroscopy has become popular, as it replaces routine laboratory analysis by an inexpensive, reproducible and non-destructive technique (Soriano-Disla et al. 2014). While the sample collection and preparation are still required, laboratory conditions allow to control for the atmospheric absorption and scattering, surface scattering, illumination geometry and shadowing. Because of the controlled conditions and repeatability, laboratory spectroscopy gives rise to the creation of soil spectral libraries. Common protocols for the collection of laboratory soil spectra are needed, such as the FAO Glosolan and the IEEE P4005 working group in development. The use of soil spectral libraries for regional/continental MRV systems is not yet developed (Nocita et al. 2014).

Field spectroscopy allows a non-invasive in-situ assessment of soil surface. Hence, contrarily to the laboratory spectroscopy, light conditions and soil surface conditions (roughness, vegetation cover, moisture, presence of exogeneous material) are not controlled for. Multiple studies (e.g. Christy (2008); Mouazen et al. (2005); Reeves (2010)) noticed a degradation of the accuracy of the method for soil property prediction in the field compared to laboratory tests.

2.3.3.2 Imaging spectroscopy

The use of remote sensing opened a new perspective in soil research and monitoring. The cost-effectiveness and large quantity of spatial data obtained through remote sensing have made it the number one technique for assessing SOC contents at larger scales (Angelopoulou et al. 2019).

Various sensor types (e.g. hyperspectral, multispectral) are mounted on either airborne or spaceborne platforms. The aforementioned platforms are differentiated in terms of their spatial, spectral and temporal resolution (Angelopoulou et al. 2019). Consecutively, the field of application and accuracy of each platform is dependent on its specifications (Angelopoulou et al. 2019).

Multispectral sensors like Landsat-8 or Sentinel-2 record a fairly limited number of discrete spectral bands (4-20 bands), while hyperspectral sensors include a very large number of contiguous and narrow spectral bands of 5-15nm (Transon et al. 2018). Therefore, the spectral quality of hyperspectral sensors is thought to produce much higher accuracy for quantitative assessment of soil properties (Gholizadeh et al. 2018).

Airborne hyperspectral sensors provide promising results in quantitative soil mapping, as they combine a high spectral resolution with a high spatial resolution, and with a relatively low atmospheric perturbation (Transon et al. 2018). However, mounting hyperspectral sensors on spaceborne platforms has seen some constraints, related to the Signal-to-Noise Ratio (SNR), and technical challenges in large data collection and transfer. Therefore, hyperspectral satellites are poorly represented in the spaceborne missions, compared to the multispectral ones (Transon et al. 2018).

The use of remote sensing techniques for soil property detection is hindered by several limitations. Independently of the platform or spectral resolution, only the surface properties can be inferred (surface layer of 0-2 mm thickness). Additionally, many conditions that cannot be controlled are included in the spectra, decreasing the quality of the bare soil signal. For instance, vegetation, straw, roughness or soil moisture alter the spectral signal from soil. The effects of the disturbing factors on SOC prediction will be the subject of section 2.4.2.

2.3.4 Multivariate analysis

The prediction of SOC from spectroscopy techniques relies on an empirical approach. Correlating the spectral signatures with soil properties is done through multivariate statistical or machine learning methods, known as chemometrics. Numerous techniques have been used to relate spectral measures to soil properties: Multiple Linear Regression (MLR), Artificial Neural Networks (ANN), Convolutional Neural networks (CNN), Regression Trees (RT), Random Forest (RF), Principal Component Regressions (PCR), or Partial Least Square Regressions (PLSR). Amongst these, PLSR stands out as the most used technique for SOC prediction with spectroscopy (Angelopoulou et al. 2019).

2.3.4.1 PLSR

The PLSR approach uses the full spectrum to establish a linear regression model with the property of interest. When large number of correlated predictor variables (in this case the electromagnetic spectra) are present, PLSR constructs a new set of principal components which are linear combination of the original variables (Geladi and Kowalski 1986). This has the advantage of avoiding co-linearity problems, which are common when the number of explaining variables (the spectral bands) is high. The principal components are determined by both the response variable (here SOC) and the predictor variables, so that the newly formed components are relevant to explain most of the variation in response variable (Geladi and Kowalski 1986). The general PLSR model has the following form (Equation 2.3) by Geladi and Kowalski (1986)):

$$\begin{aligned} X &= TP' + E \\ Y &= UQ' + F \end{aligned} \quad \text{(Equation 2.3)}$$

with Y the matrix of responses (known SOC values), X the matrix of predictors (the spectral bands), T the X-scores, P

the C-loadings, E the X-residuals, U the Y-scores, Q the Y-loadings and F the Y-residuals. The PLSR algorithm constructs components from X (TP') and Y (UQ') that maximize the covariance between X-scores and Y-scores (Geladi and Kowalski 1986). The constructed components, latent variables (LV), therefore contain the significant spectral information. The optimal number of LV is determined by minimizing the Root Mean Square Error (RMSE) (Nocita et al. 2014). This step is crucial to avoid the problem of overfitting, i.e. where model produces a very good calibration but will fail to predict samples from the validation set. This is because an increase in the number of LVs results in a decrease in the variability not accounted by the model (Pasquini 2003)

The performance of the PLSR model is assessed using the following parameters: coefficient of determination (R^2) (Equation 2.4), Root Mean Square Error (RMSE) (Equation 2.5), and Ratio of Performance to Deviation (RPD) (Equation 2.6):

$$R^2 = \frac{\sum_{i=1}^n (\hat{y}_i - \bar{y})^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (\text{Equation 2.4})$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (\hat{y}_i - y_i)^2}{n}} \quad (\text{Equation 2.5})$$

$$RPD = \frac{std}{RMSE} \quad (\text{Equation 2.6})$$

where $\hat{y}$ = predicted value, $\bar{y}$ = mean observed value, y = observed values, n = number of samples with $i = 1, 2, \dots, n$, and the standard deviation of the observed values (std). The RMSE constitutes a limit beyond which it is impossible to reliably differentiate two samples having a smaller difference in SOC content (Stevens 2008)

RPD helps to interpret the prediction ability of the model. Thresholds for RPD can be found which classify the models

into three categories: non reliable when $RPD < 1.4$, fair when $1.4 < RPD < 2$ and excellent when $RPD > 2$ (Chang et al. 2001). Minasny (2013), however, considers these thresholds to be arbitrary and lacking statistical or utilitarian basis. The RPD indicator is therefore used for comparison to the literature only.

2.4 APPLICATIONS

The first milestone in SOC mapping from remote sensing occurred in 2002 with the mapping of SOC, soil field moisture and soil salinity from DAIS hyperspectral sensor in the Izrael Valley (Ben-Dor et al. 2002). Since then, many researchers have investigated the implementation of remote sensing product for SOC prediction (see Table 2.2). The SOC maps produced by airborne imagery cover relatively large areas, generally between 200 – 500 km².

Several researchers have pointed out some of the limiting factors in airborne data for SOC prediction. Brook and Ben-Dor (2011) mentioned the sensitivity of airborne data to atmospheric correction, weather conditions and the varying quality of the sensor's stability and sensitivity. Complications with atmospheric correction and radiometric calibration were also reported by Stevens et al. (2008), who have shown a degradation of SOC model quality when switching from laboratory to airborne sensing technique. Hbirkou et al. (2012) evaluated the performance of the airborne hyperspectral sensor HyMap and reported a harmful effect of soil roughness and partial vegetation cover on SOC prediction models in field scale. Similar observations were made by Lagacherie et al. (2008) who exposed the degradation of estimation performances when going across scales and sensors, e.g. radiometric calibration, spectral resolution, spatial variability, illumination conditions, and surface status including roughness, soil moisture and presence and nature of pebbles.

SOC estimation and mapping based on spaceborne data is undergoing a significant shift since 2015. This is driven on one hand by the advances in machine learning techniques that generate better calibration models and overall better accuracy, and on the other hand by the advent of the Big earth observation data era, spearheaded by Sentinel-2 free imagery, as well as by the emergence of large fleets of small satellites (e.g., Planet Cubesats) (Angelopoulou et al. 2019). The arrival of spaceborne hyperspectral sensors, such as the Environmental Mapping and Analysis Program (EnMAP, now in commissioning phase) will provide unprecedented data streams (high spatial, spectral and temporal resolution) for the retrieval and hence monitoring of SOC, across the VNIR–SWIR spectral range (Angelopoulou et al. 2019).

Table 2.2: *Non-exhaustive review of the literature on the quantitative prediction of soil organic carbon by means of remote reflectance spectroscopy. PLSR = Partial Least Squares Regression, MLR = Multiple Linear Regression, SVMR = Support Vector Machine Regression, OLS = Ordinary Least Squares, RF = Random Forest, CB = Cubist Algorithm, GBT = Gradient Boosting Trees. S=Sentinel, L=Landsat. * References marked by an asterisk have used soil composites for SOC prediction. More on soil composite in section 2.4.1.*

Table 2.2 (continued)

Reference	EO data	Statistical method	Study area	Size (km ²)	RMSE (gC kg ⁻¹)
Airbone platform					
Ben-Dor et al. (2002)	DAIS	MLR	Israel	380	0.9
Selide et al. (2006)	HvMap	PLSR MLR	Germanv	220	2.9 2.2
Stevens et al. (2008)	AHS-160	PLSR	Belgium	52.5	1.7
Stevens et al. (2010)	AHS-160	PLSR PSR	Luxembourg	420	4.25 3.99
Bartholomeus et al. (2011)	AHS-160	SVMR PLSR	Belgium		4.87 1.65
Hbirkou et al. (2012)	HyMap	PLSR	Germany	0.18	0.76
Denis et al. (2014)	AHS-160	PLSR	Luxembourg	420	3.58 – 4.90
Baver et al. (2016)	HvMap	MLR	South Africa	320	4.3
Vaudour et al. (2016)	AISA-Eagle	PLSR	France	221	3.73 – 4.49
Castaldi et al. (2018)	APEX	PLSR	Belgium	462	1.5
			Luxembourg	146	4.9

Table 2.2 (continued)

Reference	EO data	Statistical method	Study area	Size (km ²)	RMSE (gC kg ⁻¹)
Airborne platform (continued)					
Gholizadeh et al. (2018)	CASI	SVMR	Czech Republic	0.73 – 1.76	0.06 – 0.12
Castaldi et al. (2019c)	APEX	RF	Germany	200	10.6
		PLSR	Belgium	426	1.7
		PLSR	Luxembourg	204	3.0
Ward et al. (2020)	HySpex	PLSR	Germany	13	11.88
Spaceborne platform					
Gomez et al. (2008b)	EO-1	PLSR	Australia		7.3
Castaldi et al. (2014)	EO-1	PLSR	Italy	0.29	4.1
		OLS	Italy	0.29	4.0
Diek et al. (2017)*	L5-8	MLR	Switzerland	12499	2.4
Gholizadeh et al. (2018)	SI-2	SVMR	Czech Republic	0.73 – 1.76	0.08 – 0.23
Gallo et al. (2018)*	L5	PLSR	Brazil	2420	22.3

Table 2.2 (continued)

Reference	EO data	Statistical method	Study area	Size (km ²)	RMSE (gC kg ⁻¹)
Spaceborne platform					
Castaldi et al. (2019a)	S-2	RF	Germany	10 000	6.8
Castaldi et al. (2019c)	S-2	RF	Germany	200	12.2
		PLSR	Belgium	426	1.9
		PLSR	Luxembourg	204	4.0
Vaudour et al. (2019a)	S-2	PLSR	France – Versailles	221	1.23
			France - Payne	48	3.31
Žižala et al. (2019)*	S-2	CB	Czech Republic	1.45	3.4
Žižala et al. (2019)*	L8	SVM	Czech Republic	1.45	2.8
Safanelli et al. (2020)*	L4-7	GBT	Europe		15.2
Vaudour et al. (2021)*	S-2	PLSR	France	221	2.53 – 5.45
Silvero et al. (2021)*	L8	CB	Brazil	4814.6	6.20
Silvero et al. (2021)*	S-2	CB	Brazil	4814.6	6.12
Zepp et al. (2021)*	L4-7	RF	Germany	130 000	12.4

Gholizadeh et al. (2018) stated that the SOC prediction accuracy obtained by Sentinel-2 data is generally slightly lower than that retrieved by airborne hyperspectral data, while Castaldi et al. (2019c) obtained a similar prediction accuracy with S2 data as with airborne hyperspectral data (Table 2.2). The main differences between spaceborne and airborne sensors are related to resolution (temporal, spatial, spectral and radiometric) and cost of operation (Angelopoulou et al. 2019). Due to their distance from the ground, airborne applications provide higher spatial resolution than spaceborne missions. Airborne applications also show a high flexibility on the time of the flight, however for a much higher operational cost and complexity (Angelopoulou et al. 2019). Satellite platforms on the other hand, have a pre-fixed temporal resolution, but their course cannot be altered. Their pre-fixed temporal resolution, however, can be beneficial for the creation of time series.

2.4.1 Soil Composite

Remote sensing techniques in general are highly affected by external factors, such as the atmospheric disturbance (varying with season, clouds, sun azimuth and elevation), as well as by the varying conditions of the surface of the croplands during overflight due to roughness, moisture, or crop (residue) cover. In fact, the spectrum for an important fraction of the cropland does not reflect the signal of a soil. Moreover, because of crop rotation, the area fraction of exposed soil varies with acquisition date. The combination of the soil exposure with the soil surface conditions limits the area that is likely to be correctly predicted at any given moment. This reduces the usability of remote sensing techniques in soil science, especially for generating continuous soil maps showing the spatial variation of different soil properties (Diek et al. 2017).

A noticeable change occurred when Gerighausen et al. (2012), followed by Demattê et al. (2016) and Diek et al. (2016) used multi-temporal images. They used several images from consecutive years over the same area. With this method, Demattê et al. (2016) could increase the total bare soil area from 36% in a single image to 85% for the fused image. Diek et al. (2016) applied a similar approach with airborne imaging spectroscopy data. They combined three airborne images from the same area at different dates and more than doubled the amount of bare soil pixels compared to one acquisition. These studies show that multi-temporal remote sensing can be used to increase the amount of spectral bare soil information (Diek et al. 2017).

Similarly, Diek et al. (2017), Demattê et al. (2018), Gallo et al. (2018), Rogge et al. (2018), Loiseau et al. (2019), Vaudour et al. (2021) and Castaldi (2021) created a multi-temporal mosaic. In addition to increasing the amount of exposed soils, they attempted to stabilize the reflectance spectra of the soil, by removing pixels with disturbing effects and selecting only the best representative reflectance of soils for each band. The common approach relies on the empirical definition of a spectral index threshold that is then used to discriminate between soils in suitable conditions and other types of soil surfaces. Among these indices are the normalized difference vegetation index (NDVI) (Loiseau et al. 2019; Rogge et al. 2018), bare soil index (BSI) (Diek et al. 2017), normalized burn ratio (NBR2) (Castaldi 2021; Demattê et al. 2018; Gallo et al. 2018) and Sentinel-1 (S-1) derived volumetric soil moisture per pixel (S2WI) (Vaudour et al. 2021). More on soil surface disturbing effects and spectral indices in Chapter 3.

2.4.2 Disturbing effects

As stated above, spectroscopy in outdoor conditions is constrained by atmospheric conditions, clouds, cloud shadows and spatial variation in surface soil properties. The prediction models assume that a specific soil property i.e., SOC influences the reflectance within the VNIR-SWIR (400–2500 nm) range. Therefore, other factors that also influence the reflectance spectrum will disturb the prediction of the soil chromophore in question (Vaudour et al. 2019b).

Several pre-processing techniques exist for atmospheric correction for satellite imagery (e.g. Atmospheric Topographic Correction (ATCOR) software, MAJA, sen2cor, SNAP) and for cloud and cloud shadow masking (e.g. FMask, ATSA) scenes (Li et al. 2022). While atmospherically corrected imagery is usually freely provided (e.g. Sentinel level-2A data), cloud and cloud shadow detection is an essential step in satellite image preprocessing but is not always freely available. The removal of contaminated image by shadows projected by clouds on the ground surface is a crucial step for obtaining correct soil reflectance information.

The main factors affecting the soil reflectance spectrum on the ground are soil water content, vegetation, crop residues, and soil roughness (Angelopoulou et al. 2019). On rough soils with aggregates of 20 to 25 mm, Rodionov et al. (2014) obtained an overestimation of the SOC content by 61%. Nocita et al. (2013) obtained a poor SOC prediction when they did not account for soil moisture: an RMSE of 30.21 g kg^{-1} and an R^2 of 0.25 when a calibration on dry samples was applied to moist samples. Bartholomeus et al. (2011) overestimated SOC content by $> 5 \text{ g kg}^{-1}$ at a fractional maize cover of 5% to 10%. Rodionov et al. (2016) obtained an increase in SOC content by almost 30 g kg^{-1} when 5% of the surface was covered with green leaves and straw. Hence, if SOC is to be estimated over increasingly large areas, one must either be able to verify, at a distance,

that the soil reflectance spectrum is not affected by these disturbing factors, or apply a correction for these factors.

2.4.2.1 Vegetation

The pigment in plant leaves, chlorophyll, strongly absorbs visible light (wavelength ranging from 400 to 700 nm), which is used as source of energy in photosynthesis (Carlson and Ripley 1997). By contrast, the cell structure of the leaves strongly reflects in NIR, because if absorbed, the photon energy of such wavelengths would result in overheating, and would harm the tissue (Carlson and Ripley 1997). The more leaves a plant has, the more these wavelengths of light are affected. The most common spectral index for characterizing vegetation growth is the Normalized Difference Vegetation Index (NDVI) (Rouse et al. 1974) (Equation 2.7)

$$NDVI = \frac{R_{NIR} - R_{Red}}{R_{NIR} + R_{Red}} \quad (\text{Equation 2.7})$$

where R_{red} and R_{NIR} represent the surface reflectance over ranges of wavelengths in the red ($\lambda \sim 600$ nm) and near-infrared ($\lambda \sim 800$ nm) regions of the spectrum. An NDVI threshold can be specified, which is used to discriminate soils from green vegetation. The common NDVI thresholds used in the literature for vegetation masking are 0.20 (Gholizadeh et al. 2018; Gomez et al. 2016; Lagacherie et al. 2019), 0.25 (Demattê et al. 2018; Žížala et al. 2019), 0.30 (Gomez et al. 2019; Safanelli et al. 2020) and 0.35 (Castaldi 2021; Castaldi et al. 2019a).

2.4.2.2 Crop residues

A lignocellulose absorption at 2100 nm in the reflectance spectra of crop residues has been observed due to

structural compounds such as cellulose, hemicellulose and lignin (Daughtry et al. 1996). Daughtry et al. (1996) defined a spectral variable, the cellulose absorption index (CAI), which is used for discriminating crop residues from soil. The index is based on the depth of the lignocellulose absorption feature in the shortwave infrared region (2000–2200 nm); (Equation 2.8):

$$CAI = 0.5 (R_{2.0} + R_{2.2}) - R_{2.1} \quad (\text{Equation 2.8})$$

where $R_{2.0}$ is reflectance at 2030 nm, $R_{2.1}$ at 2100 nm and $R_{2.2}$ at 2210 nm. Nagler et al. (2003) found that CAI linearly increased for crop residues ranging from 0% (bare soil) to 100% cover and concluded that CAI is relevant to situations where it is important to distinguish residues from soils. However, also the main compounds of SOM (cellulose, lignin and starch) affect reflectance around 2100 and 2300 nm (Ben-Dor et al. 1997), and they might be masked by crop residue, as both SOM and residues impact the same spectral features. Rodionov et al. (2016) established a non-linear relationship between CAI and SOC overestimation in croplands, and proposed a correction of laboratory SOC predictions using the CAI as an indicator for crop residues. A variation on the CAI index, the normalized CAI (nCAI) (Equation 2.9), has been used by Mzid et al. (2022); Ward et al. (2020) and by Chabrillat et al. (2011) in the HYPerspectral SOil MApper (HYSOMA) software interface, which is used to derive quantitative mineralogical maps using ground-truth data for field calibration:

$$nCAI = \frac{0.5 (R_{2.0} + R_{2.2}) - R_{2.1}}{0.5 (R_{2.0} + R_{2.2}) + R_{2.1}} \quad (\text{Equation 2.9})$$

Both CAI and nCAI require the use of a hyperspectral sensor with high spectral resolution, as the reflectance bands are closely spaced (2030 nm, 2100 nm and 2210 nm). Such high spectral resolution is not available for multispectral sensors mounted on satellite platforms. Both

freely available spaceborne platforms Sentinel-2 and Landsat-8, which provide an appropriate temporal and spatial resolution for SOC mapping at large scale, have a limited spectral resolution in the SWIR spectral region (2 bands: SWIR1 at 1610 nm and SWIR2 at 2200 nm), where the fingerprint of crop residues is observed. Demattê et al. (2018) used The Normalized Burn Ratio (NBR2) index calculated on the two SWIR bands of Landsat in order to remove soil spectra affected by crop residues (Equation 2.10):

$$NBR2 = \frac{R_{SWIR1} - R_{SWIR2}}{R_{SWIR1} + R_{SWIR2}} \quad (\text{Equation 2.10})$$

where R_{SWIR1} is reflectance at 1610 nm, R_{SWIR2} at 2190 nm. Castaldi et al. (2019a) used the NBR2 index on S-2 multispectral data and tested the effect of the NBR2 threshold on the performance of SOC prediction models. However, the capability of the multispectral NBR2 index for crop residue detection and soil moisture quantification still has to be proven, and no rule of thumb on NBR2 threshold selection exists.

2.4.2.3 Soil Moisture

Soil moisture drastically alters the soil albedo. The difference between the refractive index of soil and water in wet soils is smaller than for dry soils where particles are surrounded by air (Bach and Mauser 1994). The increase in refractive index with a higher level of soil moisture produces a higher scattering of incident light, which results in a larger part of light propagation, and thus absorption into the soil (Somers et al. 2010; Williams and Norris 1987). Soil reflectance decreases with increasing soil moisture, and some spectral features are more affected than others, independently of soil types (Nocita et al. 2013). The spectral range 1400-2500 nm showed generally more sensitivity to

change in soil moisture than the Vis part of the spectrum (Nocita et al. 2013; Williams and Norris 1987).

Bryant et al. (2003) developed the Water Index Soil (WISOIL) to estimate surface soil moisture based on the edges of the water band centered at 1400 nm (Equation 2.11):

$$WISOIL = \frac{R_{1.4}}{R_{1.3}} \quad (\text{Equation 2.11})$$

where $R_{1.4}$ and $R_{1.3}$ are the reflectance values at 1450 and 1300 nm.

Haubrock et al. (2010) developed the Normalized Soil Moisture Index (NSMI) to estimate surface soil moisture based on the edges of the water band centered at 1900 nm (Equation 2.12):

$$NSMI = \frac{R_{1.8} - R_{2.1}}{R_{1.8} + R_{2.1}} \quad (\text{Equation 2.12})$$

where $R_{1.8}$ and $R_{2.1}$ are the reflectance values at 1800 and 2119 nm. Soil moisture quantification and/or correction has been successfully applied on hyperspectral imagery (Bryant et al. 2003; Diek et al. 2019; Fabre et al. 2015). However, these indices are based on narrow wavelengths located in or near the water absorption bands, which are not available from spaceborne multispectral instruments. This renders their use in spaceborne multispectral satellites complex, as the indices need to be adapted per sensor and per case study, as shown by Diek et al. (2019). Castaldi et al. (2015) stated that an a priori knowledge of the soil moisture class can reduce the error of soil property estimation when using hyperspectral remote sensing data.

Synthetic-aperture radar (SAR) data in the L, C and X bands are widely used for soil moisture retrieval, and the C-band sensor carried by Sentinel-1 has demonstrated its ability to retrieve near-surface soil moisture characteristics at high

spatial resolution (El Hajj et al. 2017b; Gao et al. 2017). Nevertheless, these applications are still under development and a Sentinel-1 near-surface soil moisture product is not yet available.

NBR2 has been shown to not only react to crop residues, but also to soil moisture (Demattê et al. 2018; Yue et al. 2020). Yue et al. (2020) used a broadband spectral index approach to estimate crop residue cover with varying soil moisture contents. It needs, however, to be tested if a soil mask based on one of these indices allows the development of SOC prediction models.

2.4.2.4 Surface roughness

Irregularities in soil surfaces produce shadow areas, and the wave energy leaving these areas is many orders of magnitude smaller than energy reflected directly from illuminated soil fragments (Chabrillat et al. 2019). Baghdadi et al. (2018) found that soil roughness characteristics can be successfully retrieved from Sentinel-1 C-band in VV polarization, as long as there is prior knowledge of soil moisture content. However, a methodology that assesses the soil roughness without any prior knowledge or ground-truth data is yet to be found.

2.4.2.5 Soil crust

There are two types of soil crusts: (i) biological, which are generated from live materials such as cyanobacteria, algae, lichen and mosses and (ii) physical, which are caused by the rearrangement of soil particles as a result of the raindrop energy (Chabrillat et al. 2019). Weber et al. (2008) and Chamizo et al. (2012) developed two hyperspectral indices for detection of cyanobacteria biocrusts, being able to distinguish crust from vegetation. Ben-Dor et al. (2003) found that the effects of physical crusts on reflectance are mainly translated in a change of albedo, with absorption

features varying slightly at 1450 nm and 1900 nm. Several studies (e.g. (de Jong 1992; Eshel et al. 2004; Goldshleger et al. 2001) demonstrated that hyperspectral reflectance spectroscopy can provide a valuable method for assessing the condition of the soil crust. However, no widespread method for crust detection using spaceborne multispectral sensors is available yet, due to the atmospheric disturbance at 1450 nm and 1900 nm.

2.5 SENTINEL-2 FOR SOC MAPPING IN BELGIUM

As mentioned in the objectives of the thesis, the overall aim is to minimize or remove most of the issues that influence the SOC prediction accuracy from remote sensing. To this end, Sentinel-2 satellite mission is used, together with soil samples gathered in Wallonia, southern Belgium.

2.5.1 Sentinel-2 MSI

The S-2 mission of the EU Copernicus program has shown to be promising for soil mapping, due to its high spatial resolution, free data availability and short revisit time (Castaldi et al. 2019a; Castaldi et al. 2019b; Castaldi et al. 2019c; Gholizadeh et al. 2018; Vaudour et al. 2019a; Vaudour et al. 2019b). These studies have used the spectra of the multispectral instrument (MSI) aboard the S-2 constellation to predict SOC contents in croplands of the temperate region. The S-2 constellation is composed of twin satellites S-2A and S-2B in the same orbit but phased at 180° (Drusch et al. 2012), together providing time series with high revisit frequency (five days at the equator). The S-2 MSI has 13 spectral bands covering the Vis – NIR – SWIR spectral range (0.4–2.5 μm). Four bands have 10 m spatial resolution, six bands have 20 m resolution and two bands have 60 m resolution (Table 2.3).

Table 2.3: *Specifications of the Multispectral Instrument (MSI) on board of the Sentinel-2 constellation. Vis = visible, R-edge = red edge, NIR = near infrared, SWIR = shortwave infrared.*

Spectral band	Spectral domain	Central wavelength (nm)		Bandwidth (nm)		Spatial resolution (m)
		S-2A	S-2B	S-2A	S-2B	
B1	Vis	442.7	552.2	66	66	60
B2	Vis	492.4	492.1	36	36	10
B3	Vis	559.8	559.0	31	31	10
B4	Vis	664.6	664.9	106	106	10
B5	R-edge	704.1	703.8	15	16	20
B6	R-edge	740.5	739.1	15	15	20
B7	R-edge	782.8	779.7	20	20	20
B8	NIR	832.8	832.9	106	106	10
B8A	NIR	864.7	864.0	21	22	20
B9	NIR	945.1	943.2	20	21	60
B10	SWIR	1373.5	1376.9	31	30	60
B11	SWIR	1613.7	1610.4	91	94	20
B12	SWIR	2202.4	2185.7	175	185	20

2.5.2 Study area

With a few exceptions described in Chapter 5, the study is conducted in the southern part of Belgium, Wallonia (Figure 2.2), situated at 50°50' N and 4°00' E in Europe.

Throughout the thesis, the study area is increased from a flight strip of airborne sensor (Chapter 3, Figure 2.2), through the intersection of a single S-2 T31UFS tile with Walloon croplands (Chapter 4, Figure 2.2), to the whole Walloon region (Chapters 5 and 6, Figure 2.2). A brief overview of the main characteristics of southern Belgium is presented in this section.

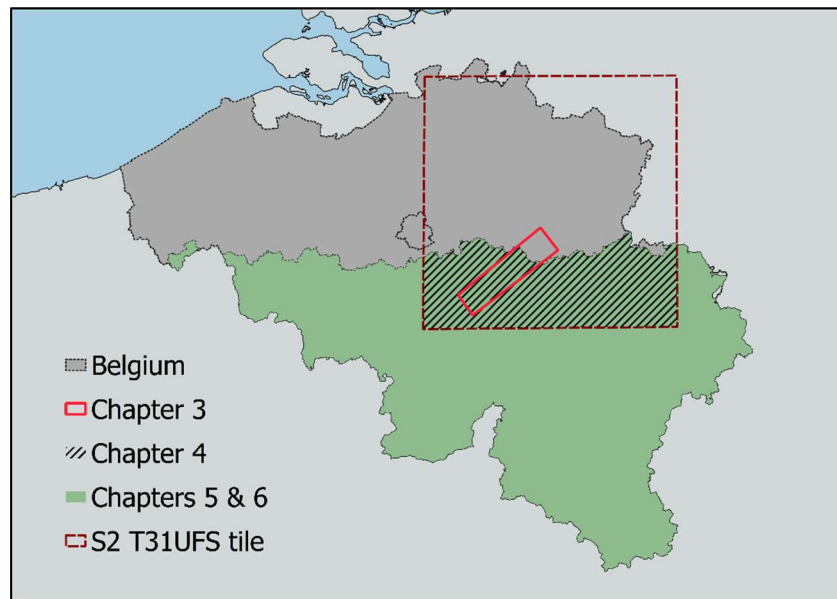


Figure 2.2: *Study area for each chapter of the thesis. Note that Chapters 5 and 6 cover the whole Walloon region.*

Belgium is segmented into 13 agricultural regions (Figure 2.3), i.e. broad zones of homogeneous characteristics in terms of agricultural practices (types of crops and livestock) and crop yields, both directly linked to soil types (texture, fertility, stoniness and drainage) and climatic characteristics (Lettens et al. 2005). The southern part of Belgium, Wallonia, covered by this study, is dominated by temperate oceanic climate. There is an increase in precipitation (from 800 to 1200 mm) and a decrease of mean annual temperature (from 10 to 8 °C) from the northwest to the southeast (Chartin et al. 2017). Sandy loam soils are dominant in the north west (haplic Luvisols, WRB (2014)), silty soils in the center and shallow silt loam and stony soils in the south east (dystric Cambisols, WRB (2014)).

A shift from intensive arable agriculture to more extensive cattle breeding can be observed along the same gradient (Chartin et al. 2017). Winter cereals, sugar beet, maize and potatoes are the dominant crops, grown in a three-year

rotation. Most soils are under conventional tillage using a moldboard plow. The croplands amount to 3878 km².

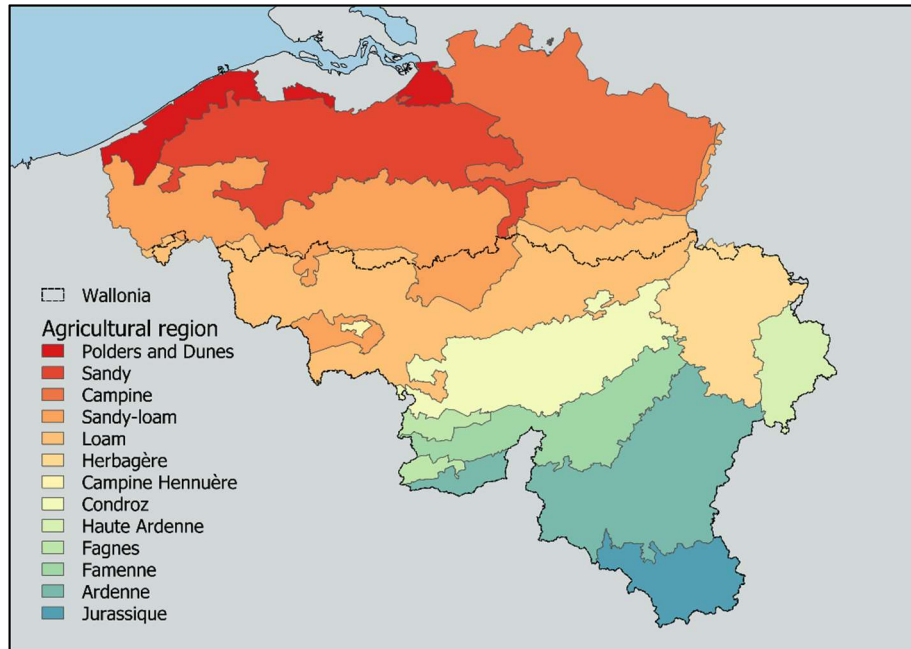


Figure 2.3: *Agricultural regions of Belgium.*

Chapters 3 and 4 focus specifically on the Loam agricultural region (Figure 2.3), because croplands are the predominant land use in the Loam belt. The dominant soils are well-drained, loess-derived haplic Luvisols (WRB 2014). The relief is gently undulating with altitudes varying between ~80m (in the north-west) and ~200m (in the south-east). The mean annual precipitation is 790 mm, with the lowest monthly mean temperature in January (2.3°C) and the highest monthly mean temperature in July (17.8°C).

2.6 CONCLUSION

This chapter presented the main factual background and concepts found in the thesis. Firstly, the importance of soils in the global carbon cycle was outlined, to better understand the context in which this thesis is inserted. The reader could

appreciate the need for the development of a cost-effective and reliable soil monitoring method, the soil being a non renewable resource essential for food security and playing an increasingly important role in sequestering atmospheric CO₂ for climate change mitigation. Fast and cheap sampling techniques are required to offer a large scale system with high temporal resolution, to detect changes in SOC. To this end, expanded use of remote sensing can help to obtain such monitoring. To understand the principles of remote sensing, this chapter elaborated on the diffuse reflectance spectroscopy. We have shown the 'fingerprint' of SOC in a soil spectrum, which will be the main lead of this investigation. We have also shown the issues of observing the SOC 'fingerprint' with proximal vs. imaging spectroscopy. While imaging spectroscopy allows to study large areas of croplands, it comes at the cost of often lower spectral resolution, and uncontrolled soil surface conditions. For instance, vegetation, straw, roughness or soil moisture decrease the performance of SOC prediction models.

We have identified a promising strategy to improve SOC prediction models using remote sensing. Removal of disturbing effects from soil pixels (mainly crop residues, moisture, crusts and vegetation) is bound to have a beneficial effect on the quality of SOC maps. This raises the following questions: (i) what is the impact of disturbing effects on SOC models, (ii) how can these disturbing effects be removed or corrected for and (iii) are the produced SOC maps from remote sensing accurate and reliable enough for their potential use in soil monitoring. The next chapters of the thesis will attempt to find an answer to these questions.

CHAPTER 3. THE EFFECTS OF CROP RESIDUES ON SOC PREDICTION FROM REMOTE SENSING¹

OUTLINE

Soil spectra are very sensitive to dry residues left at the surface of the crops after tillage, and to the soil roughness and the soil moisture content, and a meaningful calibration can only be done for smooth dry soil surfaces without residues. The objective of this chapter was to determine what are the effects of the crop residues and minimize or correct for them. This has proven to be feasible for airborne hyperspectral images with a high spectral resolution. For multispectral satellite images, however, such effects were not yet known, and there was not a clear consensus on which spectral indices are suitable to eliminate spectra affected by crop residues. The potential of S-2 imagery for this purpose was investigated in the above-mentioned pilot zone (section 2.5.2) of Belgian loam belt, and we found that NBR2 index is suitable for selecting pixels with low crop residue cover.

3.1 INTRODUCTION

Preparing for an operational earth observation platform for soil monitoring, an increasing number of pilot studies have focused on the potential of optical remote sensing techniques in SOC estimation of bare soils (Castaldi et al. 2018; Castaldi et al. 2019c; Castaldi et al. 2016; Gholizadeh et al. 2018; Guo et al. 2019; Moura-Bueno et al. 2019; Vaudour et al. 2016), Table 2.2). These pilot studies are restricted to croplands where (i) soil properties are fairly

¹ The content of this chapter was published in Dvorakova, K.; Shi, P.; Limbourg, Q.; van Wesemael, B. Soil Organic Carbon Mapping from Remote Sensing: The Effect of Crop Residues. *Remote Sens.* 2020, 12, 1913.

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uniform in the top 0–30 cm due to soil mixing during tillage, (ii) the soil is exposed and an eventual soil crust has been ploughed in before seeding, and (iii) surface water content is generally low during the cloud free sky required for useful remote sensing imagery (Chabrillat et al. 2019). As explained in section 2.4.2, spectroscopy in outdoor conditions is constrained by clouds, cloud shadows and spatial variation in surface soil properties. The prediction models assume that a specific soil property i.e., SOC influences the reflectance within the VNIR-SWIR (400–2500 nm) range. Therefore, other factors that also influence the reflectance spectrum will disturb the prediction of the soil chromophore in question (Vaudour et al. 2019b).

As mentioned in section 2.4.2, the main factors affecting the soil reflectance spectrum are soil water content, vegetation, crop residues, and soil roughness (Angelopoulou et al. 2019). For example, Bartholomeus et al. (2011), Nocita et al. (2013) and Rodionov et al. (2014), obtained poor SOC predictions when not accounting for green leaves, fractional straw cover and soil moisture (see section 2.4.2). Hence, if SOC is to be estimated over increasingly large areas, we must be able to verify, at a distance, that the soil reflectance spectrum is not affected by these disturbing factors.

The effect of crop residues on soil reflectance has been addressed in several studies. A lignocellulose absorption at 2100 nm in the reflectance spectra of crop residues has been observed due to structural compounds such as cellulose, hemicellulose and lignin (Daughtry et al. 1996) (see section 2.4.2.2). Daughtry et al. (1996) defined a spectral variable, the cellulose absorption index (CAI, (Equation 2.8)), which is used for discriminating crop residues from soil. The index is based on the depth of the lignocellulose absorption feature in the shortwave infrared region (2000–2200 nm). Nagler et al. (2003) found that CAI linearly increased for crop residues ranging from 0% (bare soil) to 100% cover and concluded that CAI is relevant to

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situations where it is important to distinguish residues from soils. However, also the main compounds of soil organic matter (SOM; cellulose, lignin and starch) affect reflectance around 2100 and 2300 nm (Ben-Dor et al. 1997), and they might be masked by crop residue, as both SOM and residues impact the same spectral features. Rodionov et al. (2016) established a non-linear relationship between CAI and SOC overestimation in croplands, and proposed a correction of laboratory SOC predictions using the CAI as an indicator for crop residues.

The S-2 mission of the EU Copernicus program has shown to be promising for soil mapping, due to its high spatial resolution, free data availability and short revisit time. The main challenge is the minimization of disturbing factors, such as residues and soil moisture on multispectral images. Demattê et al. (2018) applied different thresholds based on the Normalized Burn Ratio (NBR2, (Equation 2.10), see section 2.4.2.2) index calculated on Landsat multispectral data in order to remove soil spectra affected by crop residues. Castaldi et al. (2019a) used the NBR2 index on S-2 multispectral data and tested the effect of the NBR2 threshold on the performance of SOC prediction models. These studies have shown that the use of an arbitrary NBR2 threshold is sufficient for the goal of masking soil pixels disturbed by crop residues and soil moisture. However, no clear threshold was found yet to discriminate between soil and crop residues.

Mzid et al. (2022) have successfully demonstrated the increased SOC model performance from PRISMA hyperspectral imagery when CAI was used to remove crop residues. They used a predefined CAI threshold value for crop removal. Chabrilat et al. (2011) have developed the HYSOMA software interface, which allows an automatic generation of soil property maps based on spectral reflectance. The HYSOMA software uses normalized CAI (nCAI) to mask non-photosynthetic activity for better model

performance. The first objective of this chapter is to test the effect of a series of CAI thresholds on the performance of SOC prediction models using the Airborne Prism Experiment (APEX) hyperspectral sensor. We hypothesize that SOC prediction can be optimized by restricting the number of calibration samples by applying a CAI threshold. The second objective of this chapter is to establish whether the NBR2 calculated from the Sentinel 2 imagery can be used as a proxy for the CAI, as the latter can only be used for hyperspectral sensors.

3.2 MATERIALS AND METHODS

3.2.1 Study site and sample collection

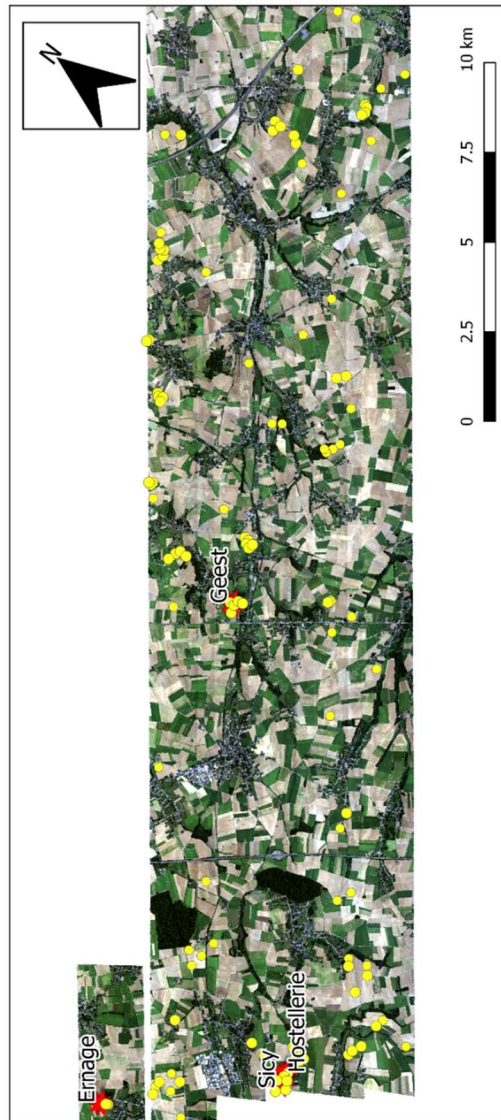
The study was conducted in an area of 240 km² located in the northern part of Wallonia, Belgium (NW: 50°35'50"N 4°39'28"E; SE: 50°42'07"N 5°06'21"E; Figure 2.2). A total of 104 surface soil samples (0–10 cm) were randomly collected in October 2018 and September 2019 (see yellow points on Figure 3.1) within fields that were without vegetation (selected based on a Normalized Difference Vegetation Index (NDVI) threshold, (Equation 2.7)) during the APEX data acquisition (2 September, 2018) (Shi et al. 2020b). These samples consisted of five sub-samples collected at random locations within a 1 m radius centered on the geographical position of a sampling plot, which was recorded by a Garmin GPS instrument with 3 m precision. The sub-samples were then thoroughly mixed and stored in a plastic bag. They were air-dried, gently crushed and passed through a 2 mm sieve. SOC was analyzed by dry combustion, using a VarioMax CN Analyzer (Elementar Analysensysteme GmbH, Hanau, Germany), as detailed in Shi et al. (2020b). For samples showing clear reactions with 10% HCl, carbonate content was measured using a modified pressure-calculator method (Sherrod et al. 2002).

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Then, SOC was obtained by subtracting the inorganic carbon content from the total carbon.

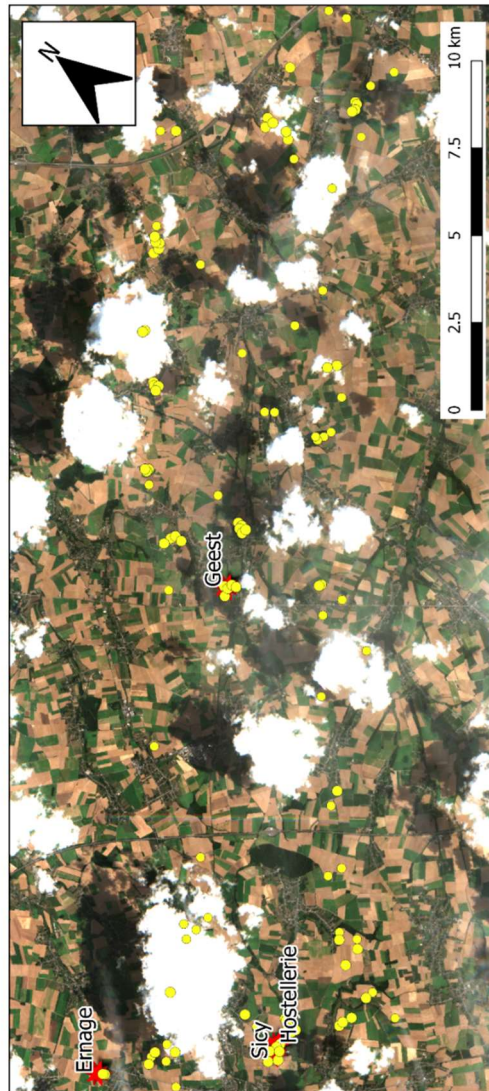
Additionally, an extra set of 276 soil samples covering three fields (Sicy, Hostellerie and Ernage; Figure 3.2) was obtained from the Walloon Agricultural Research Center (CRA-W) database. The surface soil samples (0–25 cm) were collected in August 2018 according to a regular grid (Figure 3.2). Each sample consisted of 10 sub-samples taken within a radius of 2.5 m and the latter were then thoroughly mixed for a representative sample. Sample positions were recorded using a John Deere Starfire 3000 Real Time Kinematic (RTK) GPS instrument with 2.5 cm precision. The SOC content was analyzed by means of the dry combustion method. As the two sets of samples were part of two separate campaigns, the sampling strategies were different. We, however, hypothesize that the difference in sampling depth between the two datasets of 104 samples and 276 samples (10 cm and 25 cm, respectively) do not induce a bias, as all fields are annually ploughed to a depth of c. 25 cm creating a uniform SOC content in the plough layer.

*The effects of crop residues on SOC prediction from
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(A)

*The effects of crop residues on SOC prediction from
remote sensing*



(B)

Figure 3.1: RGB image acquired by (A) the hyperspectral APEX sensor on 2 September, 2018 (red: 616 nm, green: 551 nm, blue: 470 nm) and (B) the MSI Sentinel-2 sensor on 24 August, 2018 (red: 665 nm, green: 560 nm, blue: 490 nm) in the loam belt of Belgium (see Figure 2.2 for location). The yellow dots indicate the location of the sampling points, the red stars the location of the three extensively sampled fields.

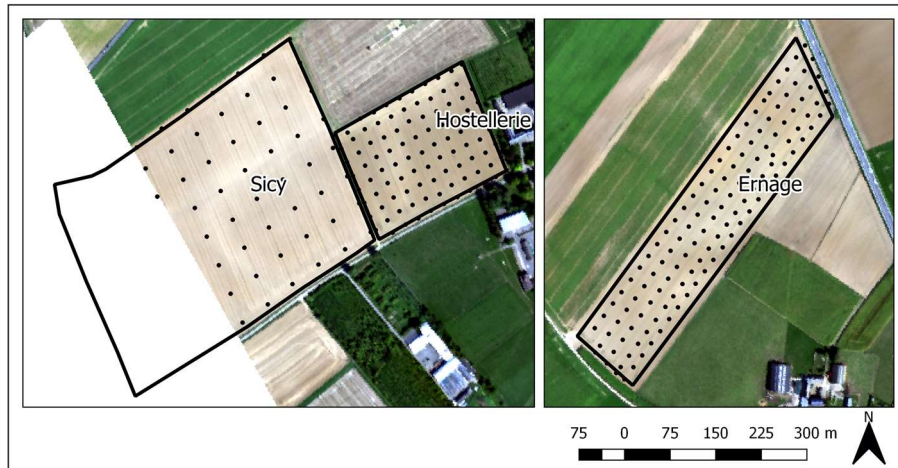


Figure 3.2: RGB image of the Sicy, Hostellerie and Ernage fields in the Belgian loam belt acquired by the hyperspectral APEX sensor on 02 September, 2018 (red: 616 nm, green: 551 nm, blue: 470 nm) and the locations of the soil samples.

3.2.2 Remote sensing data

3.2.2.1 Airborne images

A joint Swiss–Belgian airborne imaging spectrometer (APEX) acquired hyperspectral imagery on 2 September, 2018 between 10:44 and 11:56 local time in clear sky conditions (Figure 3.1A, Table 3.1). The APEX data were pre-processed at the VITO Remote Sensing Department, using the Central Data Processing Center (CDPC) for airborne Earth observation data, and are provided as georeferenced at-surface reflectance (VITO 2019). The radiometric spectral calibration was performed by means of calibration cubes generated from data measured and collected on the APEX Calibration Home Base hosted at German Aerospace Centrum (DLR) Oberpfaffenhofen and the geometric correction was based on direct georeferencing (Gege et al. 2009; Vreys et al. 2016). Noisy or troublesome bands, i.e., the water bands (1310–1555

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nm, 1750–2000 nm) and the first blue bands with poor radiometric quality (VITO 2019) (413–440 nm) were removed. For more information on the APEX imaging spectrometer, you are kindly referred to Schaepman et al. (2015).

Table 3.1: *Comparison of the MSI on board the Sentinel-2 constellation and the APEX sensor's characteristics (Drusch et al. 2012; VITO 2019).*

	MSI	APEX
Altitude (km)	786	3.6
Sensor type	multispectral	hyperspectral
Spectral range (nm)	443–2190	413–2431
Spectral bands	13	285
Resolution		
Spatial (m)	10–20–60	2
Temporal (day)	5	—
Spectral (nm)	15–180	2–13
Noisy bands (nm)	—	413–440, 1310–1555, 1750–2000
Signal to noise (SNR)		
VNIR	89:1 to 168:1	50:1 to 700:1 [8]
SWIR	50:1 to 100:1	40:1 to 600:1 * [8]

* After noisy band removal

In order to assess the quality of the APEX hyperspectral data, spectral reflectance of one black and one white reference surface were acquired at the moment of the APEX data acquisition on 2 September 2018 by means of an ASD FieldSpec portable spectral radiometer (Analytical Spectral Device Inc., USA). The spectral resolution ranges from 3 nm (at 350–1000 nm) to 10 nm (at 1000–2500 nm), and the

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spectral readings are acquired in 1 nm increments over the wavelength range. The references were a black asphalt parking lot (50°34'35.43"N; 4°42'14.7"E) and a white marl square (50°35'55.9"N; 4°50'06.7"E). The geographical position of each sampling point was recorded by a Garmin GPS instrument with 3 m precision. The sensor was positioned from the nadir approximately 1 m above the ground and the average value of nine consecutive measurements for each reference was calculated as the final spectral reference. The spectral bands from 350 to 440 nm and from 2450 to 2500 nm were removed because of instrumental noise. For comparison with airborne data, the APEX reflectance spectra were extracted for the georeferenced black and white references, using the bilinear interpolation technique. The latter assigns the output cell value by taking the weighted average of four closest cell centers based on their distance.

3.2.2.2 Spaceborne images

Multispectral field reflectance data were obtained using the multispectral instrument (MSI) aboard the S-2 platform (Table 3.1, section 2.5.1). The images were provided as Level 2A product, i.e., geometrically, radiometrically and atmospherically corrected. Since the MSI has 13 bands with different spatial resolutions, the images were spatially resampled (nearest neighbor resampling) at 10 m to maximize the level of detail of the S-2 data.

Firstly, an S-2B image with minimum cloud cover acquired on 24 August, 2018 was downloaded from the Copernicus open access hub (Figure 3.1B). The image was selected to coincide as much as possible with the APEX image. Clouds and their shadows on the S-2B image were masked using the Sentinel Application Platform (SNAP) software. The image was further geometrically registered using the airborne data as a reference image, to correct the geometrical shift of the S-2B image and thus obtain an overlap between S-2B and airborne images. Then, an S-2A

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image acquired on 13 October, 2019 was downloaded from the Copernicus open access hub, with the aim to test whether a link exists between ground-truth crop residue cover observations and the reflectance in the SWIR bands of the S-2 MSI. This date was selected because the image was cloud-free and it was acquired in autumn when many fields were bare after the harvest of potatoes and sugar beets.

3.2.3 Spectral Indices

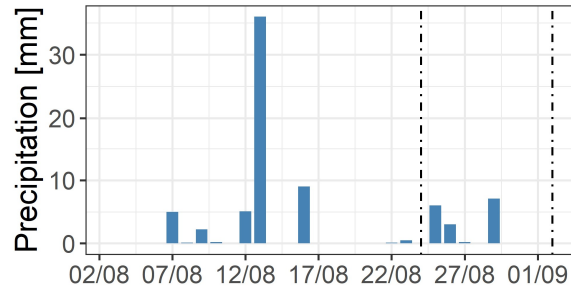
Firstly, an NDVI threshold was set to mask green vegetation (Equation 2.7). The threshold was determined by (i) visually inspecting the RGB images from the dates of overflight (Figure 3.1) and by (ii) minimizing the "salt-and-pepper" patchiness of the resulting mask. Pixels with NDVI values below 0.26 were kept for APEX, below 0.30 for S-2 (September 2018) and below 0.35 for S-2 (October 2019). Then, the wavelengths used to calculate the CAI (Equation 2.8) were somewhat adjusted, taking into account (i) the quality of the APEX airborne spectra and (ii) the theoretical positioning of the bands, which were defined by Daughtry (2001) to be centered at 2030, 2100 and 2210 nm. Finally, the NBR2 index which is calculated as the normalized difference between B11 and B12 on S-2 MSI (Equation 2.10) was used for exploiting the correlation with crop residue cover on S-2 multispectral data.

3.2.4 Weather data

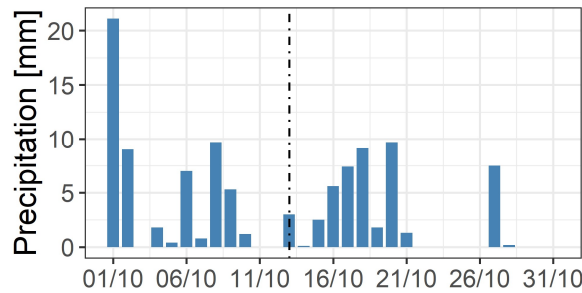
Agri4Cast weather data available for August 2018 recorded 74 mm of precipitation for August 2018 (Figure 3.3A). Moreover, during the acquisition of S-2 and APEX images dry conditions prevailed, as a dry period of at least three days preceded each image acquisition date. Additionally, daily meteorological data from the Royal Meteorological Institute (RMI) weather station Sombrefe (50°31'46"N

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4°36'03"E) were retrieved for October 2019 (Figure 3.3B). One rainy episode occurred on the day of the S-2 image acquisition (13 October, 2019) in the early morning (personal observation). This heavy rainfall occurred before the S-2 image was acquired at 10:50 local time.



(A)



(B)

Figure 3.3: (A) Daily precipitation over the Belgian loam belt study area for August 2018 and the beginning of September 2018. The vertical dashed lines represent the acquisition dates of the Sentinel-2 (24 August) and APEX images (2 September). Precipitation from weather stations was interpolated on 25 × 25 km grid. Source: Agri4Cast. (B) Daily precipitation recorded at the Sombrefe weather station in October 2019. The vertical dashed line represents the acquisition date of Sentinel-2 image on 13 October, 2019. Source: CRA-W/Réseau Pameseb.

3.2.5 Soil organic carbon predictive models

3.2.5.1 Spectral pre-processing

VNIR-SWIR spectra were extracted from the APEX images, to which the NDVI mask has been applied, at the locations of the 104 soil samples by means of bilinear interpolation technique. This method assigns the output cell value by taking the weighted average of the four closest cell centers based on their distance. The spectral matrix was passed through several pre-processing techniques, commonly used in soil spectroscopy with the aim to decrease physically related variations, remove noisy features and emphasize the important features along the spectrum (Moura-Bueno et al. 2019; Stevens et al. 2010). All pre-processing transformations were performed in "prospectr" package developed in R and the pre-treatment providing the model with the best performance was selected. The pre-treatments included: (i) absorbance (-log reflectance), (ii) 1st and 2nd order derivatives (Norris and Williams 1984), (iii) standard normal variate transformation and detrending (Barnes et al. 1989) (iv) continuum removal (Clark and Roush 1984) and (v) Savitzky–Golay smoothing (Savitzky and Golay 1964) with a window size of 20 nm and 2nd order polynomial and derivatives. In addition, all methods were calculated on (i) raw reflectance/absorbance spectra and (ii) Savitzky–Golay smoothed spectra.

3.2.5.2 PLSR model

Because a limited number of samples were available, a ten-fold-cross-validation procedure was adopted to estimate the prediction capability of the PLSR model (section 2.3.4.1) for the training set. The PLSR analyses were performed using the "pls" package developed in R software (2014). The maximum number of LV possible was set to 15. In order to detect the main spectral regions involved in the SOC prediction, the Variance Importance Projection (VIP) index

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was calculated. Spectral bands with VIP values greater than one were considered important in the PLSR model.

The performance of the prediction models was assessed using the following parameters: coefficient of determination (R^2) (Equation 2.4), Root Mean Square Error (RMSE) (Equation 2.5), and Ratio of Performance to Deviation (RPD) (Equation 2.6) of the 10-fold-cross-validation:

3.2.5.3 CAI thresholding

Several CAI thresholds (from 0.0 to 3.0 in steps of 0.25) were tested to exclude spectra affected by crop residue cover from the PLSR analysis. To ensure that the predictive accuracies of the several PLSR models based on various CAI thresholds are comparable, we must make sure that the training datasets are comparable. Vašát et al. (2017) have shown that training sets with larger variance achieve a more accurate prediction in terms of variance explained. Therefore, Levene's test ("car" package in the R Core Team, 2017) was used to verify the assumption that variances are equal across all training sets based on the CAI threshold, with a significance level of $\alpha = 0.05$. The SOC training sets partitioned by CAI thresholds were further analyzed by descriptive statistics and frequency histograms. The general overview of the modelling approach is displayed in Figure 3.4.

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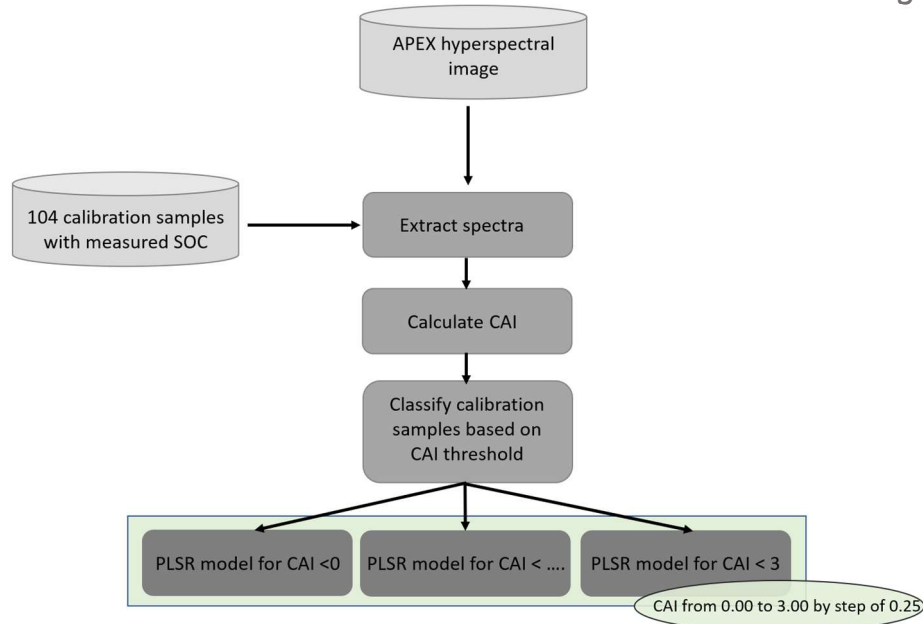


Figure 3.4: *Overview of the SOC prediction approach.*

Additionally, to evaluate the possibility of S-2 MSI for SOC prediction, we used the hyperspectral airborne data to simulate the spectral bands of S-2. The resampling of airborne data according to the S-2 bands was conducted by means of the `resample2` function in the "prospectr" package developed in R software. A PLSR model was then built on the resampled reflectance matrix in the same way as described in section 3.2.5.2. The spatial resolution and the calibration dataset were kept constant.

3.2.6 Linking CAI and NBR2

To establish a link between CAI obtained from the hyperspectral sensor and NBR2 obtained from both hyperspectral and multispectral sensors, we randomly selected a set of 188 fields with an NDVI below the threshold defined in section 3.2.3 on both the S-2 (August) and the APEX image. We manually delineated these fields, while minimizing the border effect using a 60 m buffer. Then, 70 points (to reduce computation time) were randomly placed

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within each field for which the NBR2 index was calculated on the S2 images after bilinear interpolation. For the APEX image, first, the CAI index was calculated using a buffer of 10 m around each point. Then, we resampled the APEX spectra to the spectral resolution of S-2 MSI using the function `resample2` in the "prospectr" package developed in R in order to calculate the NBR2 index.

3.2.7 Image Classification for crop residue cover quantification

A cloud free S-2A image was acquired on 13 October, 2019. Then, fields were selected to cover the range in the crop residue variability, while avoiding vegetated areas (NDVI > 0.35 on the S-2 image). We took geo-referenced (7–8 m precision) RGB images (resolution of 3024 × 4032 pixels) of the surface of 59 fields from nadir with an iPhone 8 (18 October). The photos were then analyzed using RGB thresholds in order to estimate the residue cover. For each image a classification training set was manually selected, containing 3 classes: bare soil, vegetation and crop residue. Then we used the maximum likelihood supervised classification in ArcGIS 10.4 software by ESRI. If needed, the training sets creation was repeated until the end-result was judged satisfactory when comparing the classified image and the original RGB image. Overall, 43 images were adequately classified and were kept for further analysis. A value of 100% crop residue cover was associated to four images of maize fields at senescence.

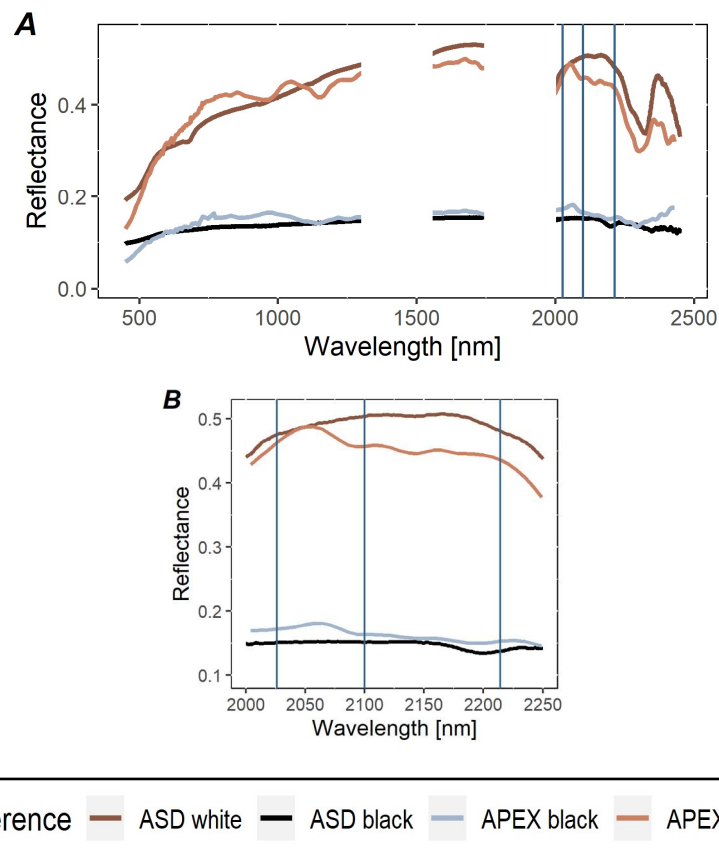
3.3 RESULTS

3.3.1 Quality of the APEX spectra

The shape of APEX spectra of the reference surfaces is marked by features not shown on the ASD spectra (peaks of reflectance at 1000 nm and around 2050 nm; Figure

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3.5A). These peaks are most probably artefacts due to the atmospheric conditions and the sensor characteristics. Remaining as close as possible to the original CAI bands and at the same time avoiding the artefacts of the APEX sensor, we selected the bands at 2026, 2100 and 2214 nm to be used in the remainder of the text (Figure 3.5B). Moreover, spectra based on the ASD field spectrometer demonstrated a slightly different albedo intensity. Hence, the CAI values obtained from the APEX spectra are to be considered as relative, and should not be compared in absolute values to CAI values measured in the laboratory. This means that we cannot use results from Nagler et al. (2003) who established a relationship between CAI and crop residue cover.



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Figure 3.5: **(A)** VNIR-SWI) reflectance spectra of black and white references recorded by the ASD pro FR portable spectroradiometer and by the APEX sensor; **(B)** zoom on the SWIR region where the soil spectra are the most affected by crop residues. The three vertical lines correspond to the cellulose absorption index wavelengths used in this study ($R_{2.0} = 2026 \text{ nm}$, $R_{2.1} = 2100 \text{ nm}$, $R_{2.2} = 2214 \text{ nm}$).

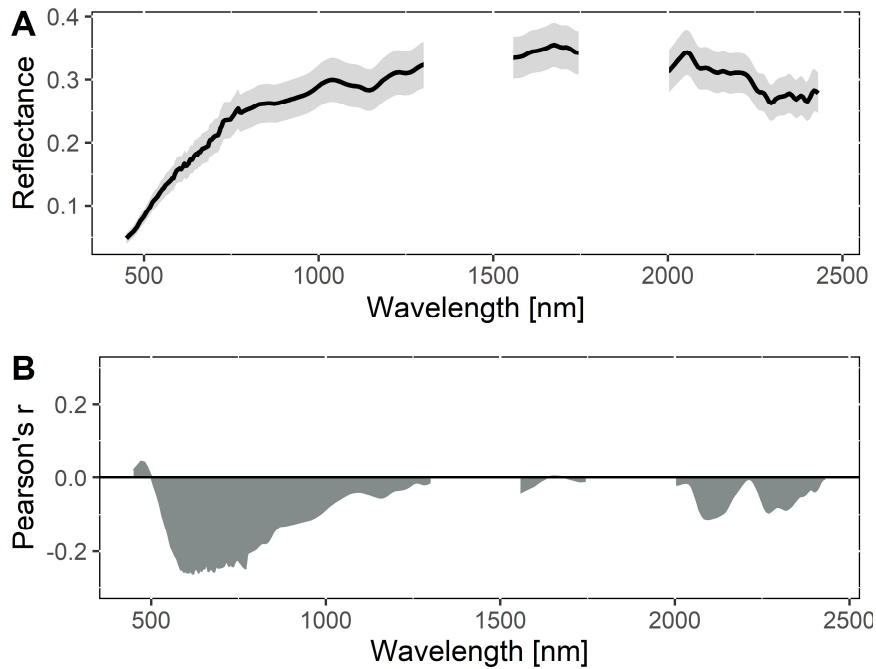


Figure 3.6: **(A)** Mean soil spectral signature (black line) and standard deviation (lower and upper boundaries) for the raw spectra of the 104 calibration samples (average SOC content 12.1 g kg^{-1}) extracted from the hyperspectral APEX sensor (image from 2 September, 2018) and **(B)** the Pearson's correlation coefficient of the soil organic carbon content with the raw hyperspectral reflectance.

The average APEX spectrum acquired from 104 pixels where soil samples were collected showed a well-defined absorption feature at 2300 nm, produced by molecular vibrations related to SOC (Figure 3.6) (Moura-Bueno et al. 2019). The relationship between SOC and the spectral

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reflectance was mainly negative ($r < 0$). The expected negative relationship between SOC and reflectance is attributed to the stretching and bending of C–H, O–H and C=C and the electronic transition portions of the electromagnetic spectrum in the VNIR region (Gomez et al. 2008a).

3.3.2 SOC prediction models

3.3.2.1 Without CAI threshold

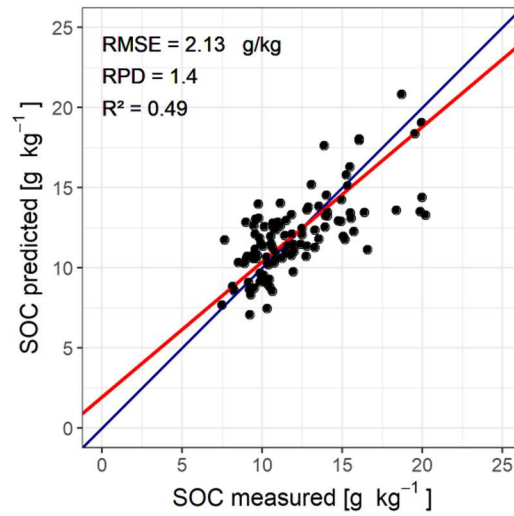
We obtained the best SOC prediction using reflectance rather than absorbance (Table A.3.1). The prediction accuracy for the ten-fold-cross validation yielded an R^2 of 0.49, an RMSE of 2.13 g kg⁻¹ and an RPD of 1.4 (Table A.3.1, Figure 3.7A). VIP values larger than one indicate the wavelength that contributes to the model overall i.e., the visible (440–740 nm), the SWIR region (2000–2060 nm and 2380–2430 nm) and in particular, the blue and green regions with wavelengths between 450 and 550 nm (Figure 3.7B). The predicted SOC content was on average 12.1 g kg⁻¹ and was rather variable (variation coefficient (CV) = 24.5%, $n = 104$, last line in Table 3.2).

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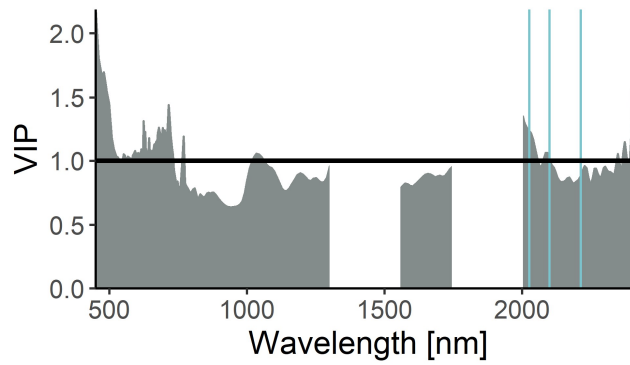
Table 3.2: Descriptive statistics of the SOC calibration dataset and the results of the PLSR model applying the CAI thresholds. In bold is the best model. CV = variation coefficient, LV = latent variables. * expressed in g kg⁻¹.

Descriptive Statistics										Ten-fold cross validation		
CAI	n	Mean *	Max *	Min *	CV (%)	Std *	RPD	R ²	RMSE *	LV		
0.00	40	10.9	16.5	7.5	19.5	2.1	1.07	0.14	1.98	3		
0.25	58	11.2	16.5	7.5	19.8	2.2	1.20	0.32	1.84	4		
0.50	75	11.5	19.9	7.5	22.4	2.6	1.38	0.48	1.87	6		
0.75	80	11.6	19.9	7.5	23.0	2.8	1.51	0.59	1.75	13		
1.00	90	11.7	19.9	7.5	23.4	2.8	1.29	0.40	2.11	4		
1.25	95	11.8	20.0	7.5	24.0	3.0	1.29	0.39	2.21	4		
1.50	99	12.0	20.2	7.5	25.0	3.0	1.30	0.45	2.31	13		
1.75	100	12.0	20.2	7.5	24.9	3.0	1.28	0.40	2.33	5		
2.00–2.50	102	12.0	20.2	7.5	24.7	3.0	1.32	0.45	2.26	12		
2.75	103	12.1	20.2	7.5	24.7	3.0	1.32	0.47	2.25	14		
3.00	104	12.1	20.2	7.5	24.5	3.0	1.39	0.49	2.13	13		

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(A)



(B)

Figure 3.7: Measured against predicted SOC in the flight line of the hyperspectral APEX. The blue line is the 1:1 line, the red line is the regression line (A) with its variance importance in projection (VIP) scores (B). Predictors with VIP values greater than one (area above the horizontal line in the plot) were considered significant for the PLSR model. The blue vertical lines show the wavelengths used for the CAI index.

The PLSR model for SOC content demonstrated sufficient accuracy to be applied on a pixel-by-pixel basis over the

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APEX image. For further model assessment, the model was firstly applied to the 276 sampling locations in three fields in the Belgian loam belt: Sicy, Hostellerie and Ernage. The three fields show a range in average CAI from 1.56 for Sicy, 0.52 for Hostellerie and 0.37 for Ernage (Figure 3.8). Student's t-test indicates (at $\alpha = 0.05$) a significantly higher CAI for Sicy field than for Hostellerie and Ernage. iPhone image taken at the day of the APEX overflight (02-09-2018) is available for Sicy field, together with the result of image classification that indicated a 24% residue cover (Figure A.3.1). The crop residue cover of the Sicy field was estimated by a supervised classification of an RGB image taken with an iPhone at the moment of APEX overflight. We observe a significant shift between the distribution of predicted and measured SOC contents in Sicy (Student's t-test at $\alpha = 0.05$ (p -value = 2.2×10^{-16}); Figure 3.8A top panel), while such a shift is not observed for the other two fields (Hostellerie and Ernage; Figure 3.8B-C top panels). The scatterplot for Sicy with the highest CAI indicates an overestimation of the SOC values (Figure 3.8A bottom panel). Such overestimation is not observed for the fields with lower CAI values (Figure 3.8B-C bottom panels).

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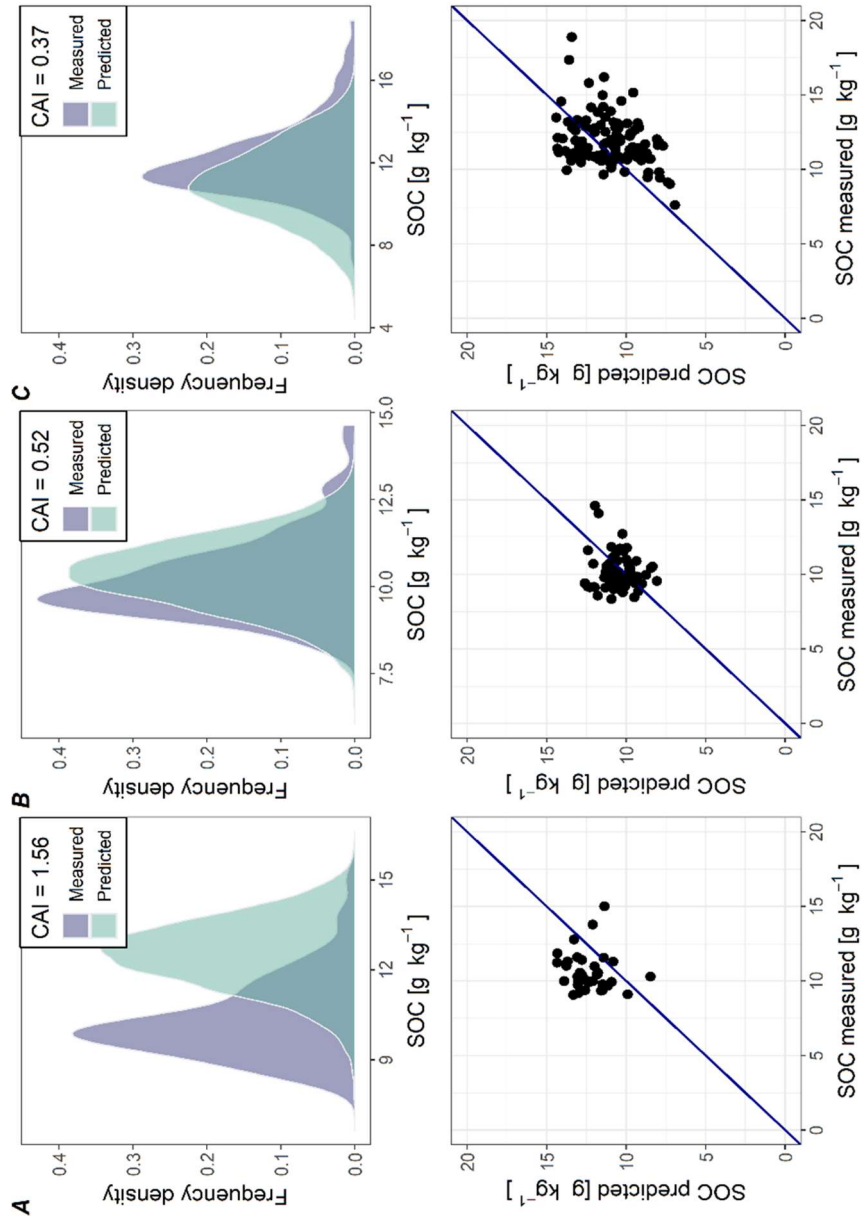


Figure 3.8: Comparison of the predicted SOC obtained from the PLSR model and the measured SOC values in the (A) Sicy, (B) Hostellerie and (C) Ernage fields, and their respective CAI values. The blue lines in the plots below are the 1:1 line. See Figure 3.1 for the location of the fields and Figure 3.2 for the location of the sampling points.

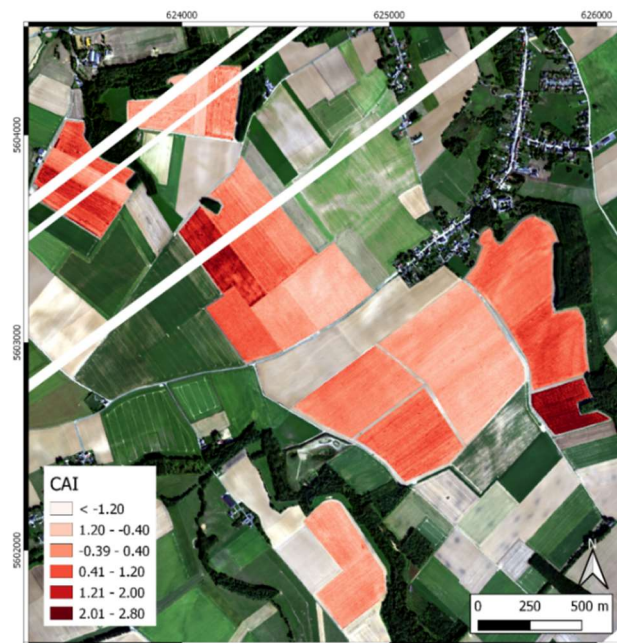
*The effects of crop residues on SOC prediction from
remote sensing*

SOC and CAI maps developed from APEX data reveal very similar spatial patterns (Figure 3.9, Figure 3.10). An area of 18 croplands with an NDVI value below the 0.26 threshold was selected in the south-eastern part of the flight strip. The SOC map mainly shows an inter-field variability of SOC with values ranging from 6.8 to 14.8 g kg⁻¹. It appears that fields with higher predicted SOC correspond to those with higher CAI values, which agrees with findings from Bartholomeus et al. (2011). SOC and CAI maps of a single field confirm this observation (Geest, Figure 3.10). The Geest field appears to have a higher crop residue cover in the north-east (Figure 3.10B). The sharp and straight edges of this pattern point to farming practices such as ploughing and seeding rather than a natural gradient in residue cover reflected by the CAI. The same sharp-edged pattern is also found for the predicted SOC content. The overestimation in SOC in fields with a large CAI value (i.e., Sicy; Figure 3.8A) and the similar spatial patterns of CAI and SOC in the Geest field (Figure 3.9, Figure 3.10) strongly suggest that a partial residue cover leads to a positive bias in predicted SOC contents.

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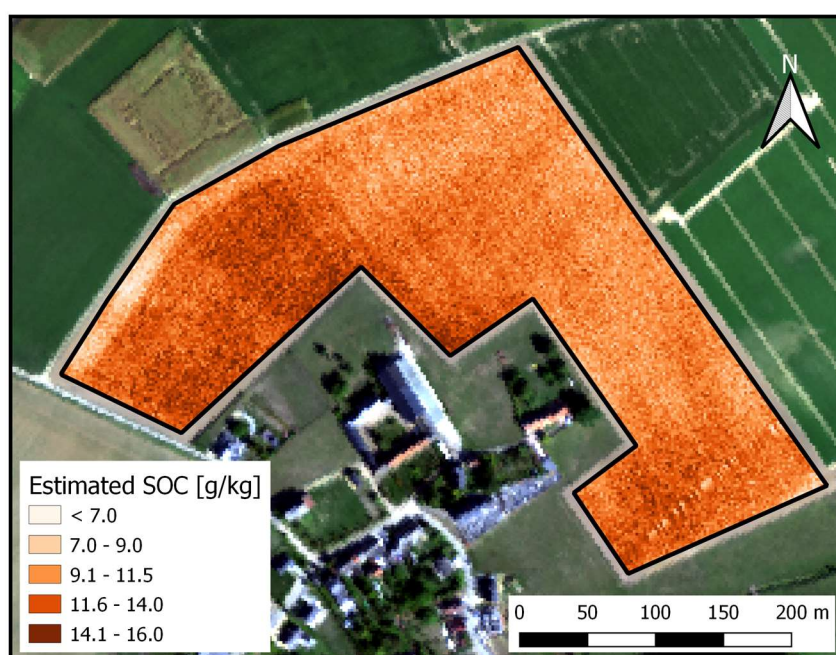
(A)



(B)

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remote sensing*

Figure 3.9: Comparison of the spatial patterns of (A) predicted SOC content by PLSR model on extracted airborne hyperspectral data and (B) the CAI calculated from extracted airborne hyperspectral data in part of the APEX flight strip. The white stripes were removed because of noise in the airborne data.



(A)

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(B)

Figure 3.10: Comparison of the spatial patterns of (A) predicted SOC content by a PLSR model on extracted airborne hyperspectral data and (B) the CAI calculated from extracted airborne hyperspectral data in Geest field. For the location of the Geest field see Figure 3.1.

We fitted an exponential model to the observed semivariance of the predicted SOC contents of 8000 random points in an area of 30 km² in the south-eastern part of the flight strip (Figure 3.11, Table 3.3). The range is reached at 335 m, the same order of magnitude as an average field size. In theory, sample locations separated by distances larger than the range are not spatially autocorrelated, whereas locations closer than the range are.

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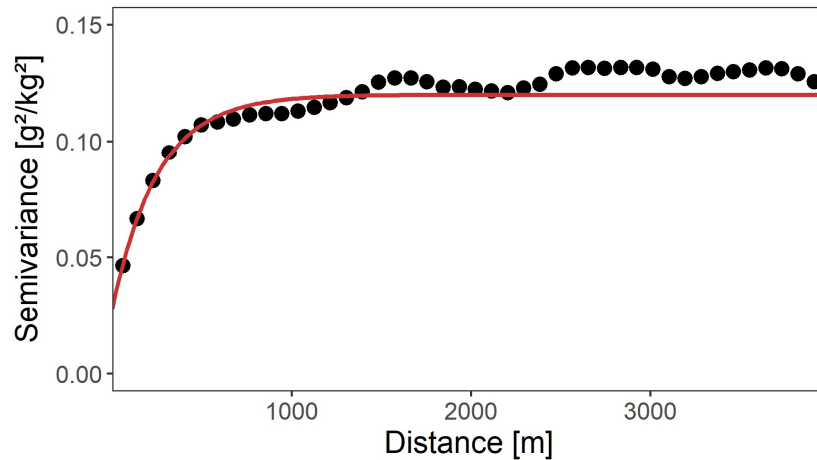


Figure 3.11: Variogram of the predicted SOC data for 8000 random locations. The points are the experimental semivariance (expressed in g^2/kg^2) values whereas the red line is the model of variogram.

Table 3.3: Variogram parameters of the fitted model (Figure 3.11) for predicted SOC obtained from a PLSR model.

Model	Sill (g^2/kg^2)	Range (m)
Nugget effect	0.023	
Exponential *	0.109	335

* The exponential model has no finite range and here is reported the practical range. It is the distance at which the variogram value equals 95% of the sill variance (Richard Webster and Margaret A. Oliver 2007).

3.3.2.2 With CAI threshold

Several CAI thresholds (from 0.0 to 3.0 in steps of 0.25) were applied to create calibration subsets on which PLSR models were built to predict SOC content (Table 3.2). The CV shows a rather stable value for all subsets (19.5 for CAI

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< 0.00 and 25.0 for CAI < 1.50). The Levene's test indicates the homogeneity of variances across the calibration subsets (Table A.3.2). All p -values were higher than the significance level of $\alpha = 0.05$, except for subset CAI < 0.00 against subsets CAI < 2.75 and CAI < 3.00. Those subsets have significantly different variances and should therefore not be compared. For future reference, a subset of equal number of samples should be created for each calibration subset for better practice, to exclude the influence of different sample sizes. The model performance varies with the CAI threshold (Figure 3.12, Table 3.2): The lowest performance is obtained if a strict threshold of CAI < 0.00 is applied. This is likely due to the low number of calibration samples ($n = 40$). The model performance then increases to reach a maximum at CAI < 0.75 ($R^2 = 0.59$, RMSE = 1.75 g kg^{-1} and RPD = 1.51). Then, model performance decreases and remains more or less stable for CAI thresholds from 1.00 to 3.00. The scatterplot for the measured and predicted SOC from absorbance spectra with a calibration subset of CAI < 0.75 is illustrated in Figure 3.13A. The dispersion of points is less marked than on the PLSR model without a CAI threshold (Figure 3.7A). Overall, similar patterns in VIP are observed with a peak in the blue and green regions regardless of the CAI threshold (Figure 3.7B and Figure 3.13B).

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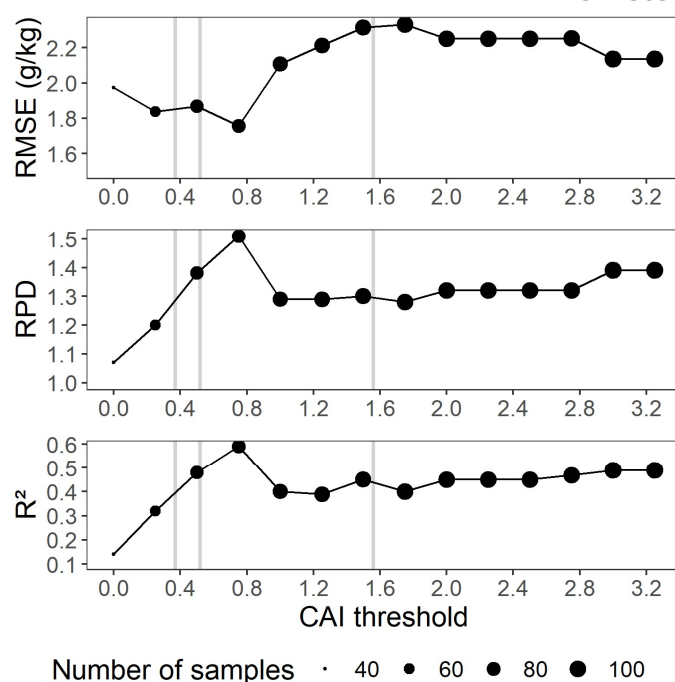
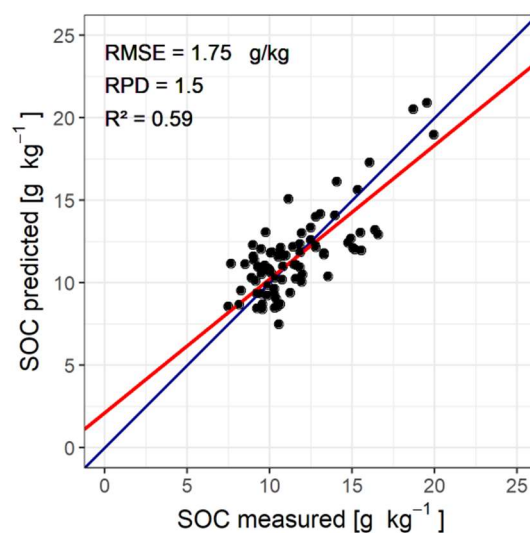
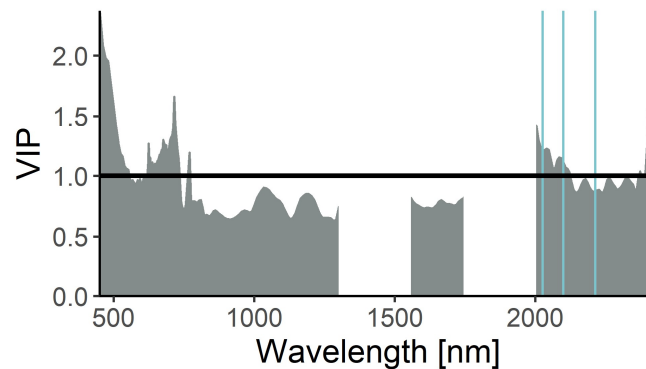


Figure 3.12: R^2 , RPD and RMSE of the PLSR models for SOC content as a function of CAI thresholds. The vertical lines indicate the average CAI values of three fields: Sicy: 1.56, Hostellerie: 0.52 and Ernage: 0.37 (Figure 3.2 and Figure 3.8).



(A)

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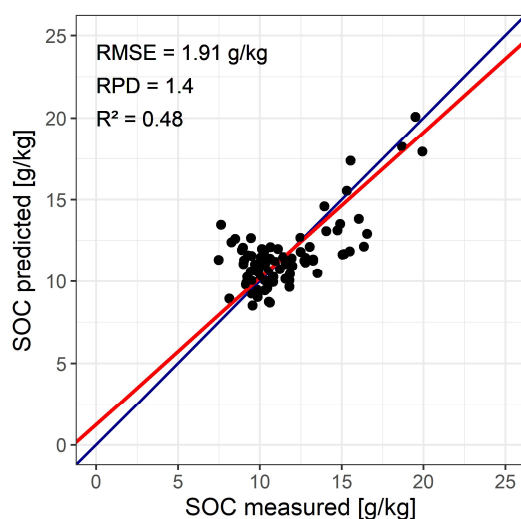


(B)

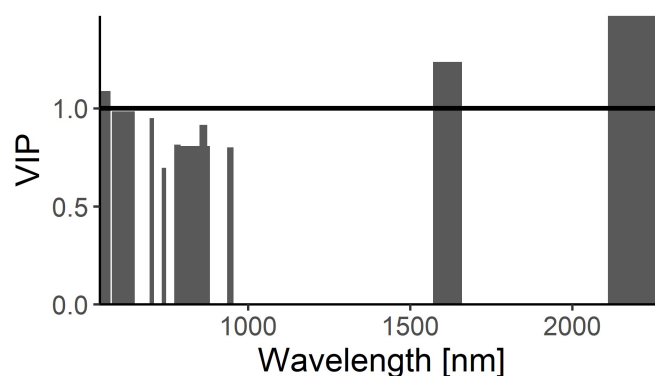
Figure 3.13: *Measured against predicted SOC in the flight line of the hyperspectral APEX sensor with a CAI threshold at 0.75. The blue line is the 1:1 line, the red line is the regression line (A) with its variance importance in projection (VIP) scores (B). Predictors with VIP values greater than one (area above the horizontal line in the plot) were considered significant for the PLSR model. The blue vertical lines show the spectral wavelengths used for the CAI index.*

The results of a PLSR model built on a reflectance matrix resampled to S-2 MSI spectral resolution are shown in Figure 3.14. The calibration subset was selected based on the CAI threshold that provided the best SOC prediction, i.e., $CAI < 0.75$. The model performance is inferior to that of the model built with hyperspectral data ($R^2 = 0.48$, $RMSE = 1.91 \text{ g kg}^{-1}$ and $RPD = 1.4$).

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(A)



(B)

Figure 3.14: Measured against predicted SOC in the flight line of the hyperspectral APEX sensor with a CAI threshold at 0.75, where spectra were resampled to Sentinel-2 radiometric resolution. The blue line is the 1:1 line, the red line is the regression line (A) with its variance importance in projection (VIP) scores (B). Predictors with VIP values greater than one (bars reaching above the horizontal line in the plot) were considered significant for the PLSR model.

3.3.3 Crop residue detection using Sentinel-2

The CAI and NBR2 values both calculated on APEX spectra from the same date show a very good linear relationship ($R^2 = 0.83$; Figure 3.15A, Table 3.4). The NBR2 index calculated on S-2 MSI and on resampled APEX hyperspectral data also shows a linear relationship (Figure 3.15B). However, a cloud of points with clearly higher NBR2 recorded on the S-2 images occurs (shaded area in Figure 3.15B). Moreover, the relationship does not follow the 1:1 line (Figure 3.15B). Therefore, the absolute values of NBR2 obtained from different platforms cannot be compared. The points in the blue shaded area of Figure 3.15B, Figure 3.15C have high NBR2 values on the S-2 image from 24 August, 2018, but lower NBR2 values on the APEX image nine days later. Hence, as high NBR2/CAI values are linked to extensive crop residue cover (Daughtry 2001; Demattê et al. 2018), we hypothesize that those are fields that have been ploughed during the nine day interval between the S-2 and the APEX images acquisition.

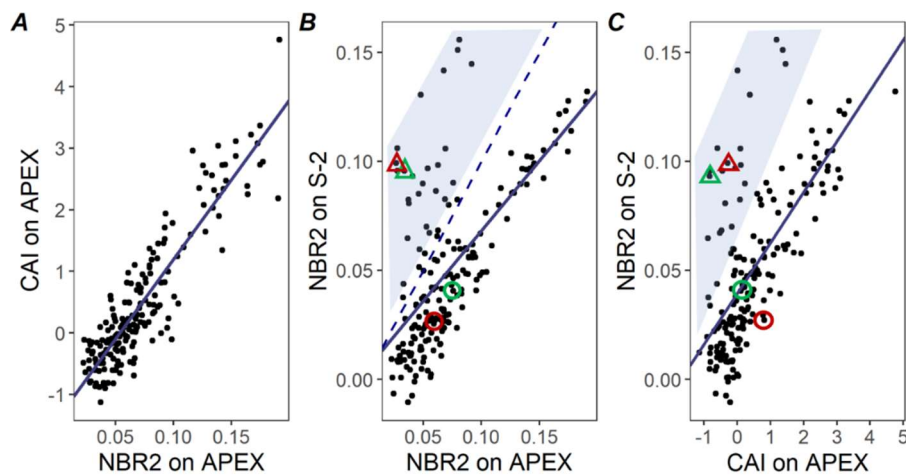


Figure 3.15: Relationships between the CAI and the NBR2 calculated on airborne hyperspectral data (APEX image from 2 September, 2018) and on satellite multispectral data (S-2 image from 24 August, 2018) on a set of 188 fields randomly selected in the Belgian loam belt. The dashed line

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in (B) represents the 1:1 line. The blue lines represent the linear regression (Table 3.4). For the explication of the blue shaded area, please see section 3.3.3. The red symbols represent fields from Figure 3.16A and the green symbols from Figure 3.16B.

Table 3.4: Linear regression models for mean values of the CAI and the NBR2 of a field calculated on airborne hyperspectral data (APEX image from 2 September, 2018) and satellite multispectral data (S-2 image from 24 August, 2018).

		Coefficients	R²	n
CAI (APEX)	Intercept	−1.403 ***	0.83	188
	~NBR2 (APEX)	Slope 25.955 ***		
NBR2 (APEX)	Intercept	0.003 ***	0.43	188
	~NBR2 (S-2)	Slope 0.642 ***		
CAI (APEX)	Intercept	0.039 ***	0.47	188
	~NBR2 (S-2)	Slope 0.023 ***		

* the significance levels are given as * p -value ≤ 0.05 ; ** p -value ≤ 0.01 and *** p -value ≤ 0.001 .

For anecdotal illustration, RGB images of two examples of neighboring fields are provided for visual inspection (Figure 3.16). The red symbols (circle and triangle) on Figure 3.15B and Figure 3.15C are the values in the fields in Figure 3.16A and the green symbols in Figure 3.15B. In each pair of RGB images, the color of one field does not change during the interval between the S-2 and APEX image (noted by a circle), while the color of the other field changes (noted by a triangle). The fields in which the color changes are those situated in the blue shaded areas in Figure 3.15B and Figure 3.15C. Based on standardized NBR2 values, the NBR2 changes from 1.3 to −1.2 (i.e., 2.5 units) for the field in the

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blue shaded area which color has changed, while for the unchanged fields, they change from -0.6 to -0.3 (i.e., -0.3 units; Figure 3.16A). Similar trends can be observed for the fields in Figure 3.16B. This however remains a speculation, as no in-situ observations are available for verification.

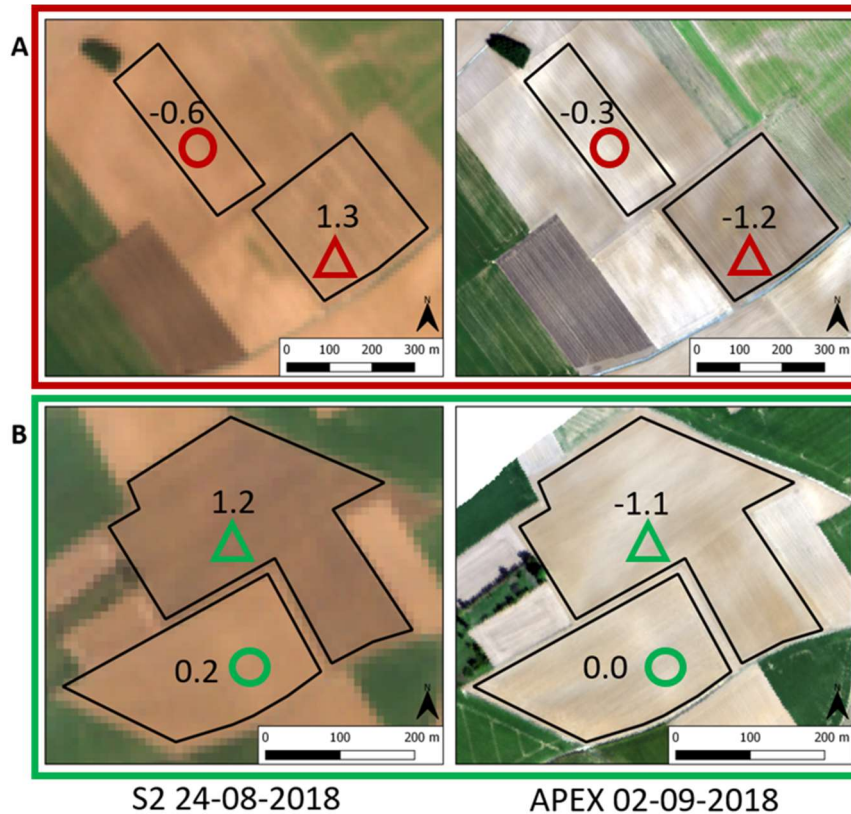


Figure 3.16: RGB images of pairs of selected fields (A and B) in the Belgian loam belt acquired by the Sentinel-2 MSI sensor on 24 August, 2018 (red: 665 nm, green: 560 nm, blue: 490 nm) (left) and the hyperspectral APEX sensor on 2 September, 2018 (red: 616 nm, green: 551 nm, blue: 470 nm) (right). The numerical values are the standardized NBR2 values extracted from Sentinel-2 MSI and resampled APEX sensor. The red (A) and green (B) circles represent fields which follow the regression lines on Figure 3.15B and Figure 3.15C, while the red (A) and green (B) triangles represent fields which do not follow the regression line, and which have likely been ploughed.

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In addition, we provide the preliminary results of a field experiment, where we test the potential of the NBR2 index based on S-2 multispectral data for estimating the crop residue cover during wet conditions in autumn. Pixels with an NBR2 comprised between 0.04 and 0.11 show no discernable trend with crop residue cover, which is lower than <15%. Pixels with a higher NBR2 (but a smaller range is observed: from 0.11 to 0.16), correspond to crop residue cover between 15% and 100%.

3.4 DISCUSSION

We have demonstrated that APEX airborne imagery is capable of predicting SOC content over a relatively large area of 240 km² dominated by croplands for which the soil surface conditions were not controlled ($R^2 = 0.49$, RMSE = 2.13 g kg⁻¹ and RPD = 1.39). The RPD might seem relatively low compared to other similar studies which reported RPD values up to 2.7 for an area in northern Germany (Castaldi et al. 2019c) and 2.39 for a north–south flight strip in Luxembourg (Stevens et al. 2010). The low RPD in the Belgian loam belt is mainly due to the small variation in SOC content (Table 3.2). Castaldi et al. (2019c) highlighted the necessity of a suitable strategy for the calibration dataset i.e., covering both the spectral variability of the area and at the same time the full range of SOC values. Considering the variability in SOC content, the PLSR model yields similar performances as reported by Castaldi et al. (2019c) and Shi et al. (2020a) for the same region. The SOC prediction maps mainly show a pattern of SOC variability between fields (Figure 3.9A and Figure 3.10A). This pattern was confirmed by the semivariogram that yields a range of 335 m corresponding to the average dimension of the fields (Figure 3.11), which means that values separated by 335 meters are not spatially autocorrelated. These results might lead to a conclusion that the region mainly shows variability between fields, likely

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related to differences in land management or land use history. Yet, when the predicted SOC distribution of three fields was compared to the measured one, we observed a significant overestimation of SOC content for the field with a high CAI index (1.56, Sicy; Figure 3.8). This overestimation was neither observed for the Hostellerie with a CAI of 0.52 nor for the Ernage field with a CAI of 0.37. Hence, the variation in SOC between fields can to some extent be attributed to the differences in residue cover during the period where fields are being prepared for seeding winter cereals.

We therefore tested different CAI thresholds for selecting the calibration samples and found an optimum at CAI = 0.75 (Table 3.2, Figure 3.12). When using a more restrictive CAI threshold (CAI < 0.75), the accuracy decreased (R^2 dropped from 0.59 to 0.14, while RMSE increased by 0.23 g kg^{-1}), most likely due to the low number of calibration samples. Hence, the optimum CAI threshold might represent a trade-off between a sufficient number of calibration samples and the purity of the pixels used for a SOC prediction model and is therefore case specific. Moreover, when a threshold of CAI < 0.75 was applied to the calibration samples, the comparison between resampled airborne data according to S-2 bands and the hyperspectral APEX data did not show a remarkable difference in terms of SOC prediction accuracy ($R^2 = 0.59$, RMSE = 1.75 g kg^{-1} and RPD = 1.51 for airborne hyperspectral versus $R^2 = 0.48$, RMSE = 1.91 g kg^{-1} and RPD = 1.40 for resampled to S-2 spectral resolution). Similar results were obtained by Castaldi et al. (2019c).

Additionally, we tested the link between CAI and NBR2. During the time of the overflight of both the S-2 and APEX sensors the soil surface was dry, as no rainfall preceded these days (Figure 3.3A) and the surface quickly dries out during the warm summer conditions. Moreover, soil roughness was generally low because fields were either in seedbed conditions or had just been harvested. The main

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disturbing factor was therefore the crop residue partially covering the soil surface. In such conditions, the CAI and NBR2 calculated on both S-2 multispectral data and resampled APEX hyperspectral data showed a linear relationship (Figure 3.15). Therefore, if we take into account the linear relationship between crop residue cover and CAI as found by Nagler et al. (2003), we can conclude that in dry conditions and on relatively smooth soils, both the CAI and NBR2 show a linear relationship with crop residue cover. However, we have illustrated that CAI and NBR2 values obtained by various platforms (laboratory, airborne or spaceborne) cannot be compared in absolute values, mainly due to atmospheric disturbance.

In order to test whether the linear relationship between NBR2 and crop residue holds when soil conditions are different, we collected photos of the soil surface in mid-autumn, after a period of heavy rainfall, and compared the residue cover to the NBR2 index. We illustrated that in such moist soil conditions, the relationship between NBR2 and crop residue cover is poor (Figure 3.17). Pixels with a variation of 0.04 to 0.11 in NBR2 had less than 15% crop residue cover, while pixels with higher NBR2 values but covering a smaller range (0.11 to 0.16) had between 15% and 100% crop residue cover. This might indicate that moist soil conditions mask the effects of crop residue cover, and/or that the effects of crop residues and soil moisture are both reflected by the NBR2 index, as has already been suggested by Musick and Pelletier (1988) and Quemada and Daughtry (2016). Indeed, Haubrock et al. (2010) defined the Normalized Difference Moisture Index (NMSI) as an indicator of soil moisture content combining reflectance values at 1800 and 2119 nm. The NBR2 index has one band at the shoulder of the water absorption band, coinciding with the NMSI band at 2119 nm (Figure 3.18). The reflectance values in S-2 bands 11 and 12 for dry, wet, and dry soil spectra with 24% residue cover (Figure 3.18) show that the difference in band 11 and band 12 is similar

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for wet soil (black curve in Figure 3.18) and dry soil with crop residues (orange curve in Figure 3.18). Hence, this combined effect of crop residues and soil moisture on the NBR2 index does not allow for a correct selection of pure soil pixels suitable for SOC prediction. Yue et al. (2020) proposed a broadband spectral angle index (BAI), which corrects for the effects of soil moisture and crop residue cover on spectral reflectance. While working on small plots, they have successfully managed to quantify maize residue cover on soils of variable moisture, using BAI on S-2 data. It remains yet to be tested if the methodology of Yue et al. (2020) can be applied to larger areas with various crop residue types.

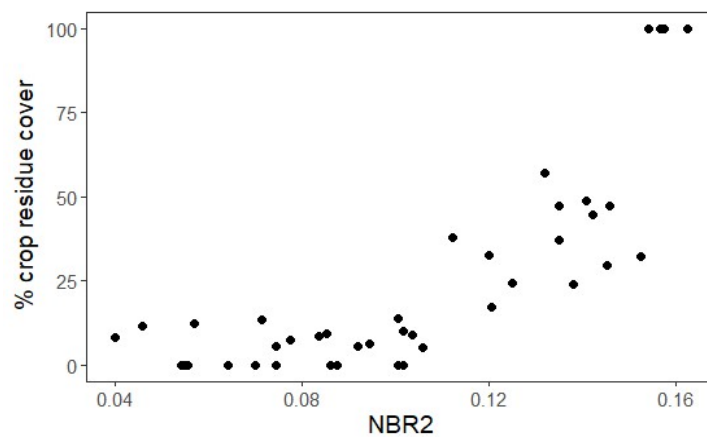


Figure 3.17: *NBR2 calculated on S-2 MSI spectra from 13 October, 2019 plotted against crop residue cover for 59 samples.*

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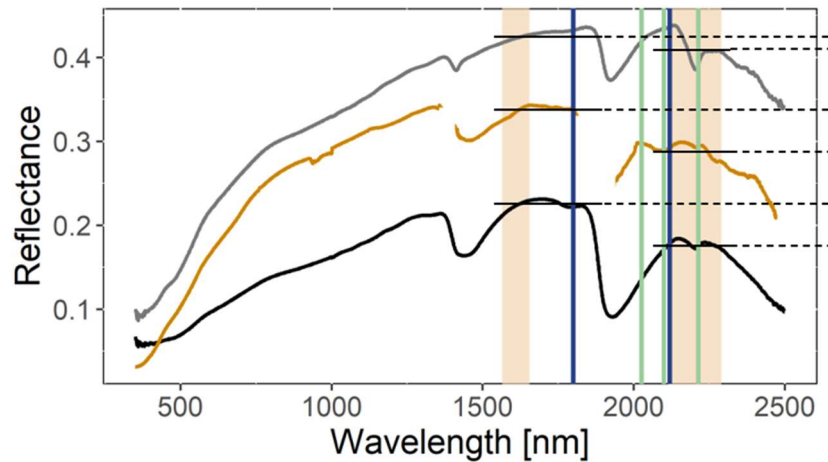


Figure 3.18: *Laboratory reflectance spectra of a dry soil sample (gray line) and a wet soil sample (black line, 25% water content), and ASD spectra of a field with 24% residue cover (orange line). The blue vertical lines indicate the position of the Normalized Soil Moisture Index (NSMI) and the green vertical lines the position of the Cellulose Absorption Index (CAI). The beige shadowed areas are the two Sentinel-2 bands 11 and 12 used for the Normalized Burn Ratio (NBR2). The black horizontal lines represent the gap between the reflectance values in the Sentinel-2 bands 11 and 12 for the three spectra.*

Vaudour et al. (2019b) demonstrated the impact of acquisition date on the prediction performance, as surface conditions vary during the growing season in function of the crop rotation. Cierniewski and Ceglarek (2018) estimated the annual bare soil distribution throughout the year in the most extensive agricultural regions, and found that for western Europe the highest amount of bare croplands, and therefore the optimal window to build SOC prediction models, occurs in mid-April and late summer to the beginning of September. In late summer, cereals have been harvested and the bare soils are likely to be dry, with stubbles on the fields that have not yet been seeded. In mid-April, some fields that have been ploughed in autumn have developed a surface crust, while other fields are seeded with summer crops. Hence, the acquisition date is a first

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indicator of the soil surface conditions, which might be encountered in an agricultural region, and thereby of the challenges to isolate pixels mimicking a soil sample as scanned in the laboratory. In this study, we have shown that in late summer, it is the crop residue effect that induces the largest error in the SOC prediction models. A similar approach should therefore be tested for the effects of soil crusts on SOC prediction models in mid-April.

Recently, many studies have focused on the use of existing datasets, such as the Land Use/Cover Area frame Survey (LUCAS) topsoil spectral library, for estimation of SOC (Castaldi et al. 2018; Nocita et al. 2014; Ward et al. 2019). Such large available soil databases allow the prediction of SOC at a low-cost with reasonable accuracy. The best results are obtained using a local regression approach where calibration samples are selected based on their spectral similarity, (Ward et al. 2019). We believe that progress in SOC mapping can be made using (i) a local modelling approach for large-scale spectral libraries and (ii) by choosing imagery acquired when the soils are, as much as possible, in the same condition as laboratory samples (i.e., smooth, dry and without residues or surface crusts).

3.5 CONCLUSIONS

We have shown that when SOC prediction models are applied to a large area without an a priori knowledge of soil surface conditions, the disturbing effects of crop residues influence the SOC prediction accuracy. In particular, an overestimation of SOC has been observed for fields with extensive residue cover. We then tested the effect of the threshold for a hyperspectral index linked to crop residues (CAI) on the performance of SOC prediction models in Belgian loam belt croplands. For dry soils in seedbed condition, the pure pixel selection based on CAI thresholds improved the SOC prediction accuracy. In particular, a CAI threshold of 0.75 allowed for the best SOC prediction model.

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Additionally, we have demonstrated that when soils are dry and in seedbed condition, CAI and NBR2 indices based on both hyperspectral airborne and multispectral satellite sensors show a linear relationship. By extrapolation, a linear relationship exists between crop residue cover and both CAI and NBR2. However, we also found that the linear relationship between NBR2 and crop residue cover does not hold when soils are wet.

CHAPTER 4. SENTINEL-2 EXPOSED SOIL COMPOSITE²

OUTLINE

As mentioned above, the soil spectra are sensitive to soil moisture, soil roughness and the presence of dry residues. While the latter has been addressed in the previous chapter, the effects of soil moisture and roughness have not. The objective of this chapter was to develop a robust method that allows selecting S-2 pixels with minimal influence of the following disturbing factors: crop residues, surface roughness and soil moisture. This was achieved by selecting the most suitable sensing period for extraction, as cultural operations have an impact on reflectance levels (Vaudour et al. 2019a). We hypothesize that there is a window in the cropping calendar, during which the surface conditions reflect the spectral signature of the soil. This occurs when soils are dry and in seedbed condition, and therefore are harrowed and without any green vegetation or crop residues. The highest likelihood for the occurrence of seedbed conditions is considered to be the last moment in the NDVI sequence, during which vegetation is on the verge of starting to grow. This is the so-called ‘greening-up’. This approach then extracts only pixels which supposedly have no crust and crop residue. An NBR2 index is then applied to filter out pixels with high soil moisture. To maximize the possible area to be predicted and to obtain an NDVI time sequence used to detect the ‘greening-up’ in time, we built image composites, which are a multitemporal mosaic of several satellite images (Rogge et al. 2018). The SOC prediction models performed on composites built using the greening-up approach performed well, and actually

² The content of this chapter was published in Dvorakova, K.; Heiden, U.; van Wesemael, B. Sentinel-2 Exposed Soil Composite for Soil Organic Carbon Prediction. *Remote Sens.* 2021, 13, 1791.

outperformed any model applied to a composite which didn't include the greening-up approach. However, the mappable area remains small (62% of croplands over a two year period).

4.1 INTRODUCTION

All studies that have demonstrated the potential of remote sensing for SOC mapping in exposed croplands (Castaldi et al. 2019a; Castaldi et al. 2018; Castaldi et al. 2019c; Chabrilat et al. 2019; Gholizadeh et al. 2018; Guo et al. 2019; Moura-Bueno et al. 2019; Vaudour et al. 2016; Vaudour et al. 2019a) have shown that the SOC prediction models are hindered by the atmospheric disturbance (varying with season, clouds, sun azimuth and elevation), as well as by the varying conditions of the surface of the croplands during overflight due to roughness, moisture, or crop residue cover, as we have shown in Chapter 3. In fact, the spectrum for an important fraction of the cropland does not reflect the pure soil signal. Moreover, because of crop rotation, which is common practice in Western Europe, the area fraction of exposed soil varies with acquisition date. The combination of the soil exposure with the soil surface conditions limits the area that is likely to be correctly predicted at any given moment.

Several authors suggested increasing the predicted area by stacking several multi-temporal images (Demattê et al. 2018; Diek et al. 2017; Gallo et al. 2018; Loiseau et al. 2019; Rogge et al. 2018; Safanelli et al. 2020; Vaudour et al. 2021). Such a multi-temporal mosaic image, or composite image, (i) allows building a more continuous map of exposed soils as it increases the amount of observed exposed soil and (ii) stabilizes the reflectance spectra of the soil (see section 2.4.1). The common approach relies on the empirical definition of a spectral index threshold that is then used to discriminate between soils in suitable and unsuitable conditions. Among these indices are the

Sentinel-2 exposed soil composite

normalized difference vegetation index (NDVI) (Loiseau et al. 2019; Rogge et al. 2018), bare soil index (BSI) (Diek et al. 2017), normalized burn ratio (NBR2) (Demattê et al. 2018; Gallo et al. 2018) and Sentinel-1 (S-1) derived volumetric soil moisture per pixel (S2WI) (Vaudour et al. 2021).

Vaudour et al. (2021) used various products for temporal mosaicking of S-2 images to predict SOC in croplands in northern France. They used an S-1 derived volumetric soil moisture separately or in combination with NDVI, NBR2, BSI and S2WI. Overall, the best trade-off between predicted area and model performance was obtained when applying the S-1 derived index to eliminate moist soils. They were able to map 40% of the cropland surface from 13 S-2 spring images acquired over two years for an area characterized by a four year crop rotation with a good result ($R^2 \sim 0.5$, RPD ~ 1.4 , RMSE $\sim 3.7 \text{ g kg}^{-1}$). Their study suggests that a number of exposed soil mosaics based on several indicators (moisture, bare soil, roughness, etc.), preferably in combination, might maintain acceptable accuracies for SOC prediction whilst covering a larger area than single-date images (Vaudour et al. 2021). However, they used an S-1 derived moisture index, which is not readily available and its computation is complex. Moreover, the calculation of this index requires a priori information on the soil moisture condition (El Hajj et al. 2017a). Additionally, timelines of SOC prediction models of Vaudour et al. (2019b) have shown an overall seasonal trend where model performance is positively correlated with solar elevation, thus suggesting that spring images might be favored compared to autumn and winter images in the Northern Hemisphere. Hence, selecting an appropriate image acquisition date might be more important for increasing model performance than the application of an index to discriminate pixels with disturbing effects.

In this chapter, we propose to use a number of indices, which are easy to compute and which can be obtained from

a single satellite i.e. the S-2 MSI (NDVI and NBR2). The NBR2 index (see section 2.4.2.2, and the work in Chapter 3) has been so far mainly used as indicator for dry crop residues firstly for Landsat 8 by Demattê et al. (2018), and later for S-2 (B11 and B12) by Castaldi et al. (2019a). However, as B11 and B12 of the S-2 MSI cover a broad SWIR range, they are not only strongly correlated to crop residues, but also to soil moisture (Musick and Pelletier 1988). In Chapter 3 we have shown that this limits the sensitivity of the NBR2 to detect crop residues on moist soils. We therefore chose to combine NDVI and NBR2 thresholds with an automatic selection of appropriate image acquisition dates based on the crop phenology: the -so-called 'greening-up' method. The methodology is inspired by the green-up and green-down processes described by Liu et al. (2020), who used these to define cropping cycles. Here, greening-up is defined as the instant where the crop has been or will shortly be sown but has not yet emerged. We introduce this principle for developing exposed-soil composites, because it is during seedbed conditions that the soil surface is in optimal conditions for spectroscopic analysis of its SOC content: (i) an eventual crust and crop residues have been ploughed in and (ii) soils have been harrowed and smoothed. Furthermore, as hardly any crop residues are left on the soil surface at the greening-up stage, the NBR2 index can be used to remove pixels affected by water. We believe that the selection of acquisition date based on development of the cropping calendar provides a more reliable index and is easier to accomplish than empirically defining thresholds for multiple spectral indices used in combination.

4.2 MATERIALS AND METHODS

4.2.1 Study site and sample collection

The study was conducted in the northern part of Wallonia, Belgium. We focus on the croplands in a 110 km × 33 km rectangle (Figure 2.2), i.e. an intersection of S-2 tile T31UFS and the croplands extracted from the Land Parcel Information system for Wallonia in 2019 (<http://geoportail.wallonie.be>). The rectangle, which covers a total extent of 3630 km², comprises 1440 km² of cropland (Figure 4.1), and covers mainly the loam belt region. The 104 surface soil samples described in section 3.2.1 were used, completed by an additional dataset of 33 samples collected and analyzed following the same methodology. In total, 137 surface soil samples were available.

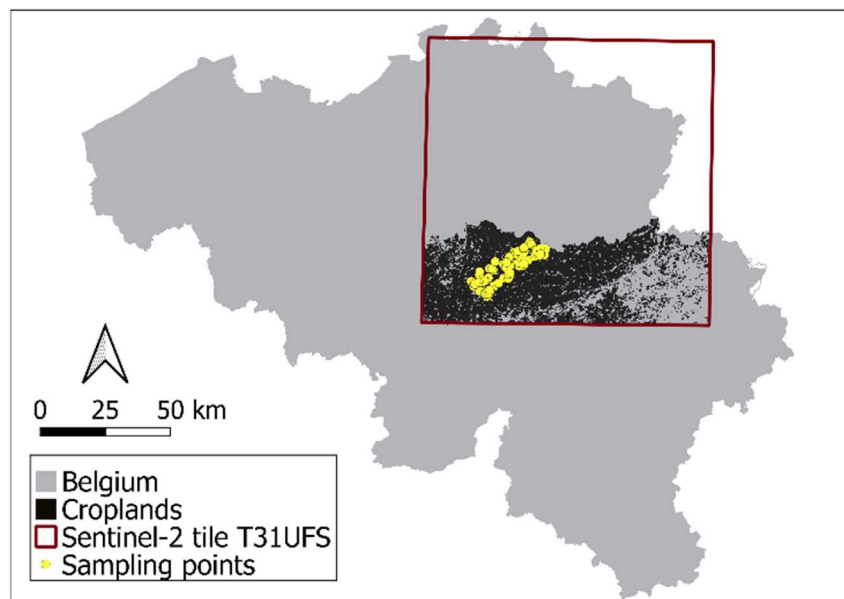


Figure 4.1: *Location of the S-2 tile T31UFS covering a large part of the Belgian loam with the sample points for calibration and validation (source of the cropland dataset: Service public de Wallonie).*

4.2.2 Remote sensing data

Spectra were obtained using the MSI aboard the S-2A and S-2B platforms (Table 2.3, section 2.5.1). A cloud-free time series composed of 36 images from 1st January 2019 to 31st December 2020 was obtained from the French land data center (<https://theia.cnes.fr>). For each date, ten bands (B2, B3, B4, B5, B6, B7, B8, B8A, B11 and B12) with correction of slope effects were provided as Level-2A product, i.e. geometrically, radiometrically and atmospherically corrected by means of the MACCS-ATCOR Joint Algorithm (MAJA) processor. Since the MSI has bands with different spatial resolutions, the images were spatially resampled (nearest neighbor resampling) at 10 m to maximize the level of detail of the S-2 data. The images were then masked using the Walloon cropland map (<http://geoportail.wallonie.be/catalogue/81bdf8bc-5968-4fd3-84ca-6be011cddd6.html>).

4.2.3 Spectral indices

A set of spectral indices was calculated for each S-2 acquisition date: NDVI (Equation 2.7) and NBR2 (Equation 2.10). Values range between -1 and 1, where higher values of NDVI indicate high green vegetation coverage. Choosing a threshold NDVI value is required for masking green vegetation. The common NDVI thresholds used in the literature for vegetation masking vary based on geographical location and soil type among others, and are 0.20 (Gholizadeh et al. 2018; Gomez et al. 2016; Lagacherie et al. 2019), 0.25 (Demattê et al. 2018; Žižala et al. 2019), 0.30 (Gomez et al. 2019; Safanelli et al. 2020) and 0.35 (Castaldi 2021; Castaldi et al. 2019a). In this chapter, the threshold was determined by (i) visually inspecting the S-2 RGB images and by (ii) minimizing the ‘salt-and-pepper’ patchiness of the resulting mask. Overall, pixels with NDVI values above 0.25 were considered as pixels containing

green vegetation. This threshold was kept constant for all 36 S-2 images.

In Chapter 3 we have shown that when soils are dry, NBR2 follows a linear relationship with crop residue cover, however in the case of moist soils, no correlation with residue cover could be found. We therefore assume that NBR2 reacts both to crop residues and soil moisture, where high values of NBR2 indicate soils that are moist and/or are covered by crop residues, but we do not make any assumptions about the form of this relationship. Hence, as setting a threshold for NBR2 index might be erroneous without relevant field observation, we chose four arbitrary classes of NBR2: (i) no threshold, (ii) below 0.15, (iii) below 0.10 and (iv) below 0.07. Additionally, weekly meteorological data from the Royal Meteorological Institute (RMI; <https://www.meteo.be/en/brussels>) weather stations Ernage and Bierset were retrieved for January 2019 until December 2020. These data were used to compare the response of NBR2 to rainfall events.

The NDVI and NBR2 indices are used here to detect soils that are likely to be exposed. Without field observation, however, it is not possible to ensure that these soils are in fact exposed. For the sake of simplicity, the 'exposed soil' terminology is used to describe soils with NDVI and NBR2 indices below the selected thresholds, suggesting that they are likely to be exposed.

4.2.4 Methods for creating composites of exposed soils

The first step was generating NDVI and NBR2 layers for each of the 36 cloud-free S-2 images using (Equation 2.7) and (Equation 2.10). An NDVI threshold obtained by expert judgment (section 4.2.3) was then applied to the NDVI layer, which was converted into 0 and 1. Hence, pixels with $NDVI \leq 0.25$ were reclassified to value 0, and pixels with

Sentinel-2 exposed soil composite

NDVI > 0.25 became 1. The binary NDVI layer and NBR2 layer were then stacked chronologically, in BinaryNDVI_{stack} and NBR2_{stack}. Any manipulation that results in the formation of a composite was performed on BinaryNDVI_{stack} and NBR2_{stack}, until the final extraction of S-2 MSI spectra for the selected exposed soil pixels. This significantly reduced the processing time. The S-2 reflectance data for pixels that respect the conditions given by the composites were extracted for bands B2, B3, B4, B5, B6, B7, B8, B8A, B11 and B12, forming full S-2 spectra. If multiple dates per pixel were selected, the S-2 reflectance data were averaged by band, in order to obtain one final spectrum.

4.2.4.1 Spectral indices-only approach

The first approach implies that the pixels to be used in the final composite image are selected on a date-independent basis, solely based on a selected threshold value of NDVI and/or NBR2 indices. Overall, five composites based on spectral indices only were proposed (i.e. A-E in Figure 4.2):

Driven by the lowest NBR2 value amongst a S-2 time series (Composite A).

Firstly, for each pixel, S-2 acquisition dates where BinaryNDVI_{stack} equals 0 were kept. An NBR2 value per date was then extracted per pixel, resulting in a vector of 36 NBR2 values for each pixel of the image. Amongst these values, the date with the lowest NBR2 value was maintained for a given pixel.

Driven by NDVI threshold value only (Composite B).

For each pixel, S-2 acquisition dates where BinaryNDVI_{stack} equals 0 were kept.

Sentinel-2 exposed soil composite

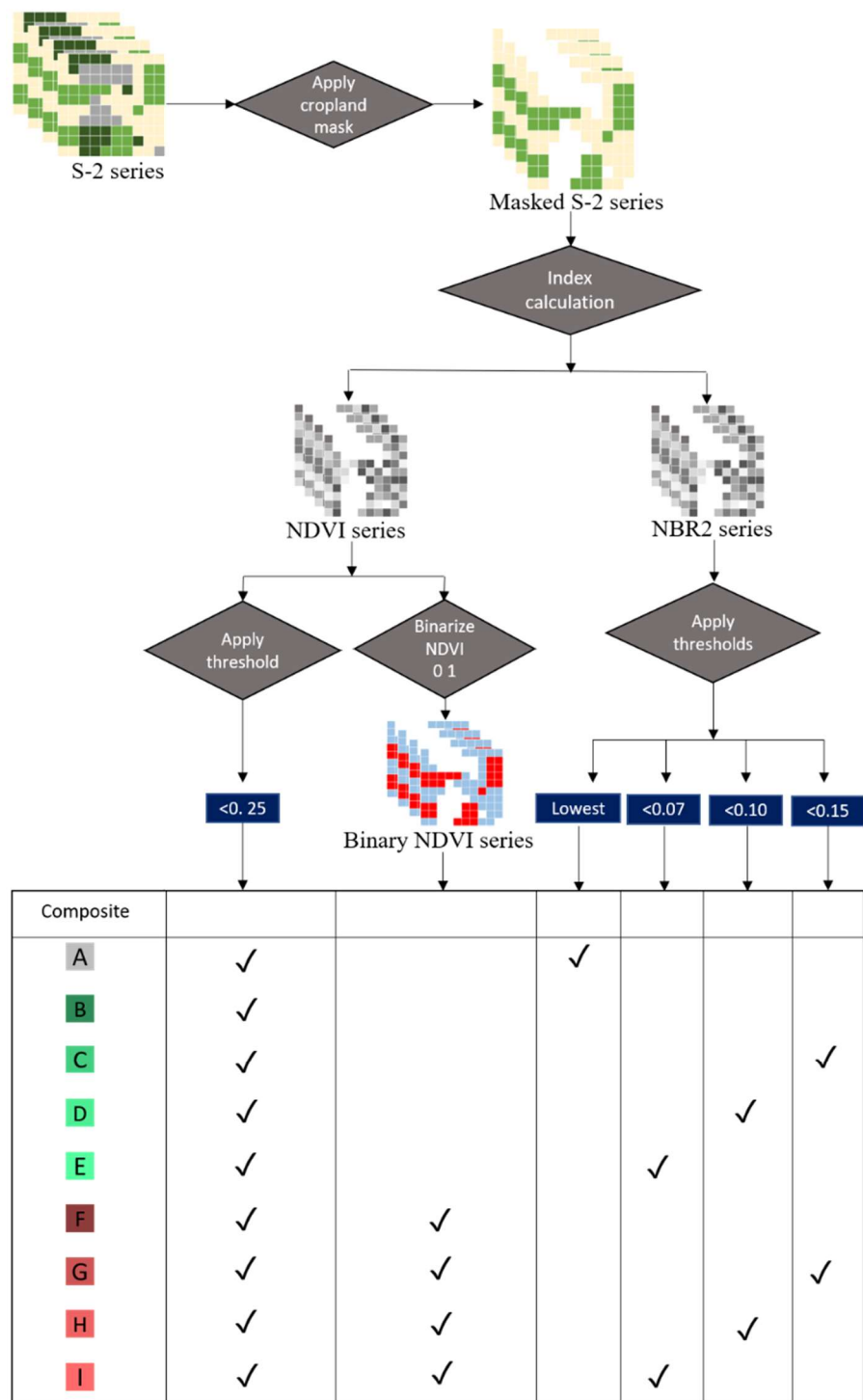


Figure 4.2: General flowchart for the composite making approach

Sentinel-2 exposed soil composite

Driven by NDVI and NBR2 threshold values (Composite C, D and E).

Firstly, for each pixel, S-2 acquisition dates where $\text{BinaryNDVI}_{\text{stack}}$ equals 0 were kept. Then, for a given pixel, NBR2 information was extracted for those selected dates from $\text{NBR2}_{\text{stack}}$. In the next step, $\text{NBR2}_{0.15}$, $\text{NBR2}_{0.10}$ and $\text{NBR2}_{0.07}$ randomly chosen thresholds were applied for composites C, D and E respectively, where any S-2 acquisition dates where NBR2 value was above the specified thresholds, were eliminated.

4.2.4.2 Greening-up approach

The greening-up approach relies on the assessment of the temporal sequence of NDVI binary values. The pixels to be used in the final composite image were selected based on the cropping calendar. We hypothesize that a window exists in the cropping calendar, during which the surface conditions reflect the spectral signature of the soil. This occurs when soils are dry and in seedbed condition, and therefore are harrowed and without any green vegetation or crop residues. The highest likelihood for the occurrence of seedbed conditions was considered to be the last moment in the NDVI sequence, during which vegetation is on the verge of starting to grow (Figure 4.3). Mathematically, this is translated as the intersection of the NDVI curve with the threshold selected for exposed soils (here $\text{NDVI} < 0.25$) *before* the NDVI reaches a local maximum (e.g. t_5 in Figure 4.3). We propose another four composites based on the greening-up approach (combined with a NBR2 index; i.e. F-I in Figure 4.2).

Sentinel-2 exposed soil composite

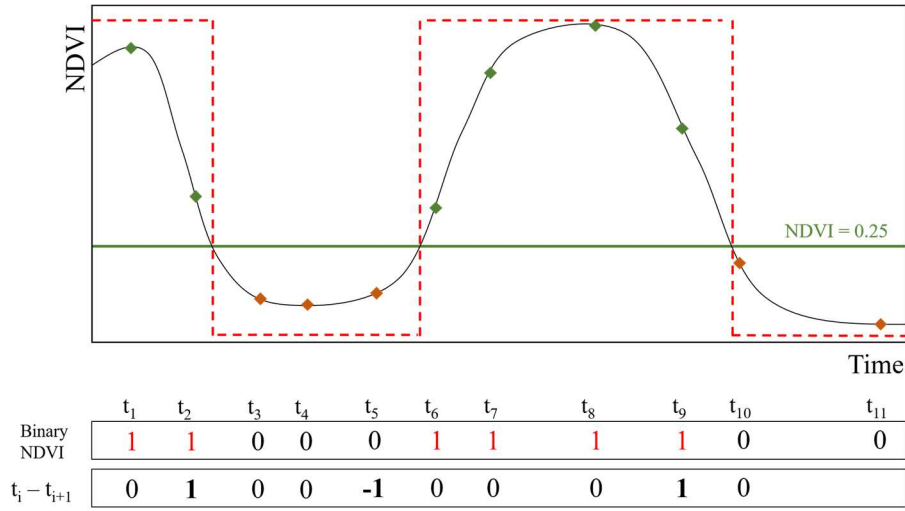


Figure 4.3: *Illustration of the recognition of the greening-up moment based on an NDVI time series. The points indicate an imaginary satellite image acquisition, the black curve is the shape of an ideal NDVI evolution of a cropland. The red dashed line is binary representation of NDVI: $NDVI \leq 0.25$ becomes phase 0 (red points), $NDVI > 0.25$ becomes phase 1 (green points). In this case, point at t_5 is considered to be at the greening-up stage.*

Driven by the Greening-up approach (Composite F, in Figure 4.2).

For each pixel, temporal sequence of NDVI binary values was extracted from $BinaryNDVI_{stack}$ (Equation 4.1).

$$BinaryNDVI_{t_i} - BinaryNDVI_{t_{(i+1)}} \quad (\text{Equation 4.1})$$

where $t \in [1, T]$ is an image acquisition date, and hence varies from 1 to 36. Each t_i for which Equation 4.1 equals -1 (see Table 4.1 for combinations) was considered as greening-up. In order to avoid false greening-up stages which are caused by a short-term increase in NDVI which does not result in a full cropping cycle, a lower limit was applied to the length of a cropping cycle. Here, the length of the cropping cycle was set as the duration (in days) which separates the instant t_i when (Equation 4.1) is equal to -1 until the instant t_i at which (Equation 4.1) is equal to 1 (in

Sentinel-2 exposed soil composite

this order). If this time period was shorter than 50 days, we excluded the selected greening-up point. This threshold is modifiable based on the regional phenology. The S-2 spectra for a given pixel were then extracted from the S-2 image acquired at t_i which was detected to be a greening-up moment.

Table 4.1: *B.NDVI = BinaryNDVI for exposed soil (0) and for vegetation (1) and the combinations obtained when applying Equation 4.1. Exposed soil followed by vegetation (which is considered here as the so-called greening-up moment) has value -1.*

$B.NDVI_{t_i}$	$B.NDVI_{t(i+1)}$	$B.NDVI_{t_i} - B.NDVI_{t(i+1)}$
Exposed soil (0)	Exposed soil (0)	0
Vegetation (1)	Exposed soil (0)	1
Vegetation (1)	Vegetation (1)	0
Exposed soil (0)	Vegetation (1)	-1

Driven by the Greening-up approach combined with NBR2 threshold value (Composites G, H and I, in Figure 4.2).

The greening-up was applied, in combination with an NBR2 index threshold value. In such way, we select pixels in seedbed conditions, and with hardly any crop residue cover. The NBR2 index is then applied to eliminate moist soils. For each selected t_i , the NBR2 value was extracted from $NBR2_{stack}$ for a given pixel. NBR2 arbitrary thresholds $NBR2_{0.15}$, $NBR2_{0.10}$ and $NBR2_{0.07}$ were applied for composites G, H and I respectively. If the NBR2 value was above the specified thresholds, the greening-up detected at t_i was eliminated.

4.2.5 Composite surface cover

It is important to characterize the fraction of the cropland area that is bare soils for each of the composites. We selected 18,000 points on each S-2 composite in order to

diminish the processing time. The points were created within the intersection of the S-2 T31UFS tile with the dataset of Walloon croplands, so that only croplands are included (Figure 4.1). A stratified random sampling method was applied to the soil association map (1:250 000, *Service Public de Wallonie*; <http://geoportail.wallonie.be>) in order to create a representative set of points. The presence or absence of exposed soil was calculated for each of the 18,000 points on composites A to I (Figure 4.2).

4.2.6 Spectral models for SOC prediction

VNIR-SWIR spectra were extracted from the S-2 images for all 36 acquisition dates at the locations of the 137 soil samples by means of bilinear interpolation technique (Figure 4.1). This method assigns the output cell value by taking the weighted average of four closest cell centers cell centers based on their distance. Any extreme values among the four cell values were not checked, however spectra with Mahalanobis Distance larger than 3 to the average spectra were removed.

SOC prediction by date.

For each S-2 acquisition date, four calibration subsets were created with (i) all samples with $NDVI \leq 0.25$, (ii) all samples with $NDVI \leq 0.25$ and $NBR2 < 0.15$, (iii) all samples with $NDVI \leq 0.25$ and $NBR2 < 0.10$ and (iv) all samples with $NDVI \leq 0.25$ and $NBR2 < 0.07$.

SOC prediction by composite.

Nine subsets of calibration samples were extracted under the constraints applying to each of the composites described above (section 4.2.4 and Figure 4.2).

The partial least squares regression (PLSR) model was then chosen to construct SOC prediction models based on the selected set according to the criteria (Figure 4.2) from the total sample set ($n=137$). The PLSR analyses (see

section 2.3.4.1 for more details) were performed using the 'pls' package developed in R software (2014). The maximum number of LV possible was set to five.

The quality of model fit was assessed using the following parameters: coefficient of determination (R^2) (Equation 2.4), Root Mean Square Error (RMSE) (Equation 2.5), and Ratio of Performance to Deviation (RPD) (Equation 2.6) of 10-fold-cross-validation.

Additionally, each set of calibration samples was subject to bootstrapping to stabilize the prediction model performance. Bootstrapping consists of repeatedly calculating a given statistic from a series of subsamples obtained by randomly resampling with replacement an initial dataset (Efron and Tibshirani 1993). Hence, for each set of calibration samples, 100 PLSR models were created and the final model performance corresponds to the mean of the 100 created models.

Several subsets of calibration points were selected for the S-2 composites to exclude unsuitable spectra from the PLSR analysis. To ensure that the predictive accuracies of various PLSR models fit to each S-2 composite are comparable, we have used Levene's test to verify the assumption that variances are equal across all training sets with significance level of $\alpha=0.05$ (see section 3.2.5.3). The SOC training sets were further analyzed by descriptive statistics and frequency histograms.

4.3 RESULTS

4.3.1 PLSR models for single S-2 acquisition dates

The SOC content was on average 12.3 g kg^{-1} and was rather variable: variation coefficient ($CV = 27.3\%$; $n=128$; Table 4.1). The prediction accuracy of PLSR models was variable (Figure 4.4): worst model performance was

Sentinel-2 exposed soil composite

obtained for 05-08-2020 when no NBR2 threshold was applied ($R^2 = 0.08 \pm 0.3$, $RMSE = 3.47 \pm 0.23$ g C kg⁻¹ and $RPD = 0.1 \pm 0.0$, $n=71$), while the best was obtained for 22-03-2019 with NBR2 threshold 0.07 ($R^2 = 0.78 \pm 0.13$, $RMSE = 0.45 \pm 0.11$ g C kg⁻¹ and $RPD = 2.7 \pm 0.9$, $n=21$). The application of the various NBR2 thresholds did not always improve the model performance for a given acquisition date. In some cases, however, the model performance yielded much better results (R^2 increased by a factor eight for the image from 05-08-2020 when no NBR2 threshold was compared with an NBR2 of 0.07). Note that when less than 20 calibration samples were available, models were not assumed stable and the PLSR results are therefore not shown.

4.3.2 PLSR models for S-2 composites

Overall, nine S-2 composites were built, which were used to select calibration subsets for the PLSR models (Figure 4.2). The CV shows a rather stable value for all subsets (min 22.8% for composite H; max 27.3 % for composites A, B and C). The Levene's test indicates the homogeneity of variances across the calibration subsets (Table A.4.1). All p-values were higher than the significance level of $\alpha=0.05$, except for composite G against composites A, B and C. These subsets have significantly different variances and should therefore not be compared. The model performance varies with composite type (Figure 4.5, Table 4.2). Composite I yields satisfactory results ($R^2 = 0.54 \pm 0.12$, $RMSE = 2.09 \pm 0.39$ g kg⁻¹ and $RPD = 1.68 \pm 0.45$), while the model performance of the other composites is poor ($R^2 < 0.20$).

Sentinel-2 exposed soil composite

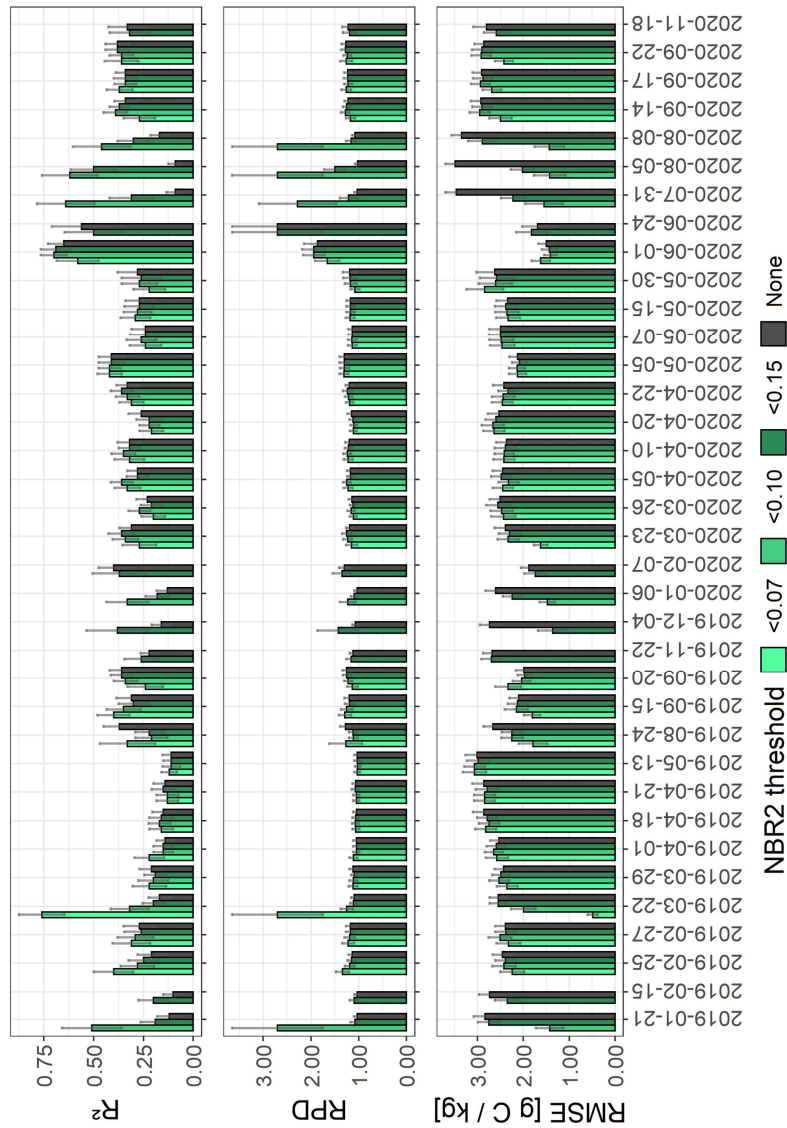


Figure 4.4: R^2 , RPD and RMSE of the PLSR models applying the NBR2 thresholds according to Sentinel-2 acquisition date between January 2019 and December 2020. Note that because of a low number of calibration samples (<20), some results are not provided.

Sentinel-2 exposed soil composite

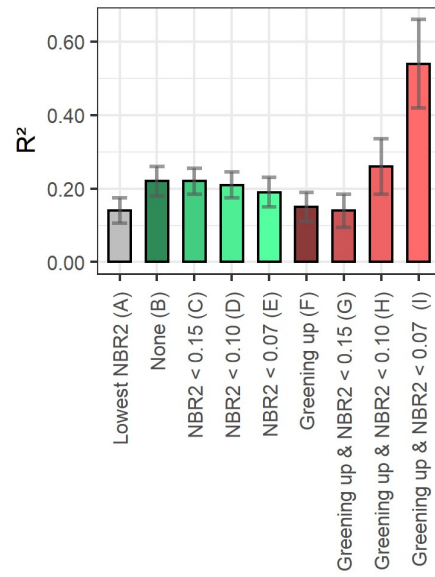
Table 4.2: *PLSR with 10-fold cross-validation applied to the Sentinel-2 derived composites. In bold is the best model. n=number of calibration samples. *expressed in g kg⁻¹*

Composite	Criteria	Descriptive statistics				
		CV(%)	STD*	Mean*	Max*	Min* n
A	Lowest NBR2	27.3	3.4	12.3	22.1	6.7 128
B	NDVI < 0.25	27.3	3.4	12.3	22.1	6.7 128
C	NDVI < 0.25 & NBR2 < 0.15	27.3	3.4	12.3	22.1	6.7 127
D	NDVI < 0.25 & NBR2 < 0.10	26.6	3.2	12.2	22.1	6.7 126
E	NDVI < 0.25 & NBR2 < 0.07	25.4	3.1	12.1	21.4	6.7 123
F	Greening-up	25.4	3.1	11.7	20.2	7.4 108
G	Greening-up & NBR2 < 0.15	22.9	2.7	11.6	20.2	7.4 91
H	Greening-up & NBR2 < 0.10	22.8	2.7	11.6	20.2	7.4 68
I	Greening-up & NBR2 < 0.07	25.7	3.2	11.3	20.2	8.0 49

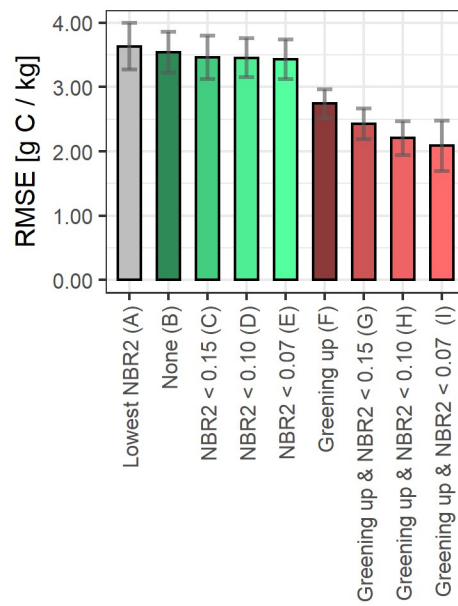
Table 4.2 (continued)

Composite	Criteria	Tenfold-cross-validation		
		RPD	R ²	RMSE*
A	Lowest NBR2	1.06 ± 0.06	0.14 ± 0.03	3.63 ± 0.36
B	NDVI < 0.25	1.12 ± 0.07	0.22 ± 0.04	3.54 ± 0.32
C	NDVI < 0.25 & NBR2 < 0.15	1.12 ± 0.06	0.22 ± 0.04	3.46 ± 0.34
D	NDVI < 0.25 & NBR2 < 0.10	1.12 ± 0.06	0.21 ± 0.04	3.45 ± 0.30
E	NDVI < 0.25 & NBR2 < 0.07	1.10 ± 0.07	0.19 ± 0.04	3.43 ± 0.31
F	Greening-up	1.06 ± 0.08	0.15 ± 0.04	2.74 ± 0.23
G	Greening-up & NBR2 < 0.15	1.06 ± 0.08	0.14 ± 0.05	2.43 ± 0.24
H	Greening-up & NBR2 < 0.10	1.14 ± 0.08	0.26 ± 0.08	2.21 ± 0.27
I	Greening-up & NBR2 < 0.07	1.68 ± 0.45	0.54 ± 0.12	2.09 ± 0.39

Sentinel-2 exposed soil composite



(A)



(B)

Figure 4.5: (A) R^2 and (B) RMSE of the PLSR models applied to Sentinel-2-derived composites based on various criteria.

Sentinel-2 exposed soil composite

The number of calibration samples available for the various composites dropped greatly for the combination of the greening-up approach with NBR2 thresholds: for the strictest NBR2_{0.07} threshold (composite I), only 49 samples were available, compared to more than 120 samples for composites A to E (Table 4.1). Mainly the spring to early autumn acquisition dates provide calibration points for the greening-up composite I (Figure 4.6).

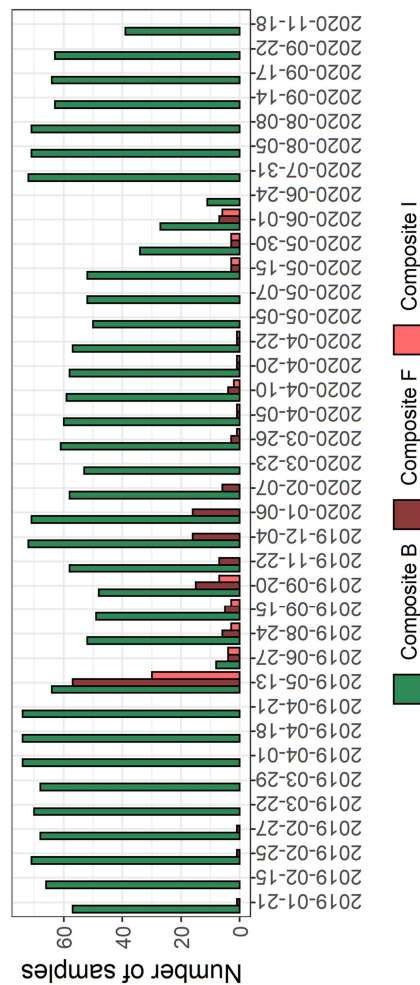
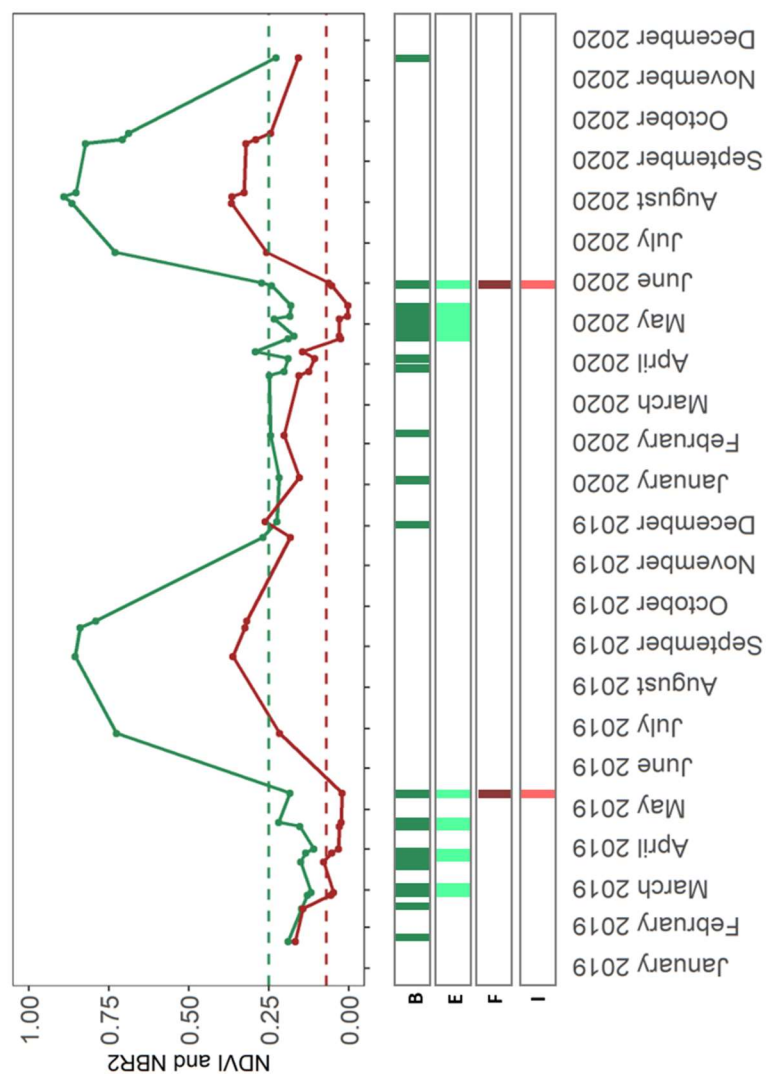


Figure 4.6: Evolution of the number of calibration samples available for each Sentinel-2 cloud-free image between January 2019 and December 2020 based on the composite criteria selection strategy.

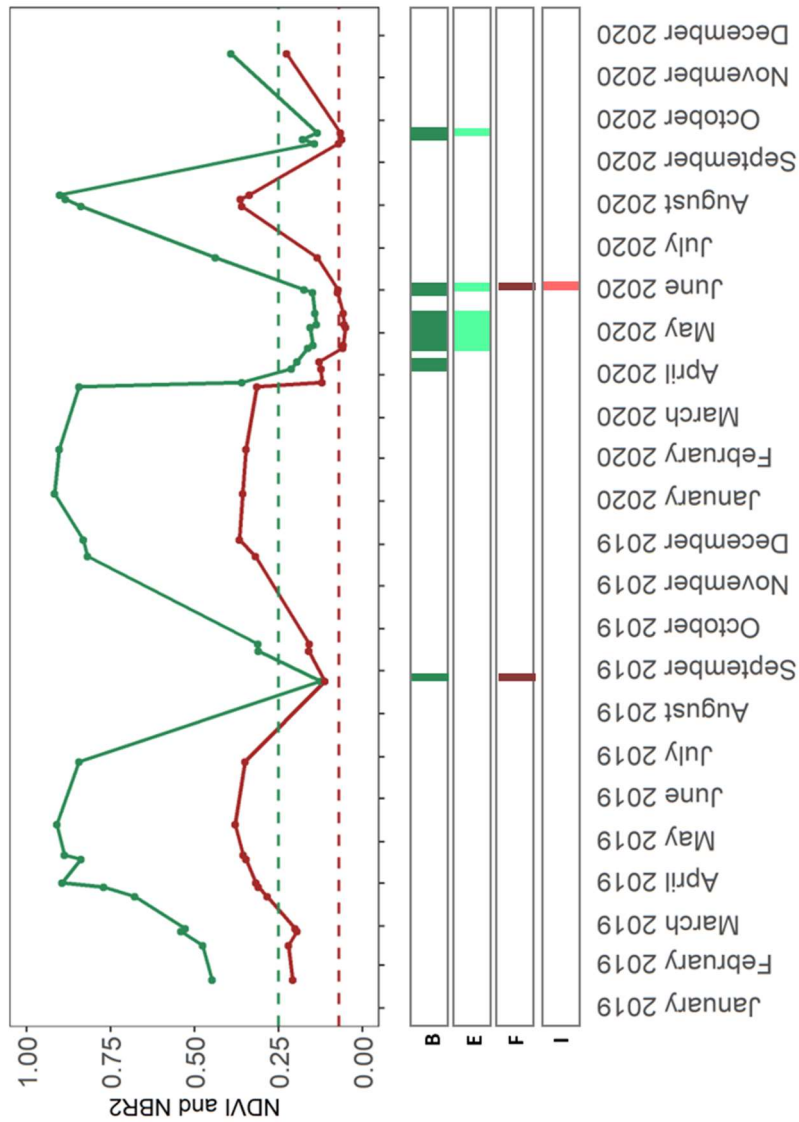
Sentinel-2 exposed soil composite

An example of NDVI and NBR2 time series from January 2019 to November 2020 is provided for two pixels (Figure 4.7). The main crop type in 2019 is maize (Figure 4.7A) and winter wheat (Figure 4.7B). The selection strategy for the dates to be included in composites B, E, F and I is also shown (Figure 4.7). It highlights the narrowing down of the acquisition date selection. The same point (example of Figure 4.7B) is included 13 times in composite B, while only once in composite I.



(A)

Sentinel-2 exposed soil composite



(B)

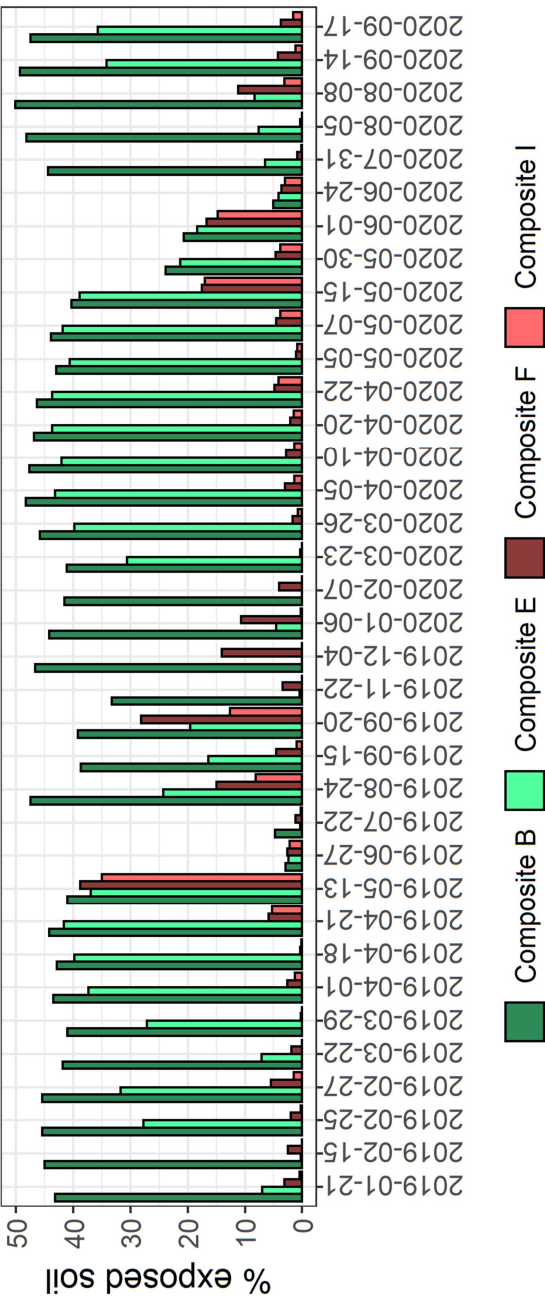
Figure 4.7: Normalized difference vegetation index (NDVI, in green) and Normalized burn ratio (NBR2, in red) series for two pixels: maize field in 2019 (A) and winter wheat field in 2019 (B). The colored vertical bars represent the inclusion of the point in the composite B, E, F or I (for interpretation of the composites see Table 4.2 and Figure 4.2). The dashed horizontal lines are NDVI=0.25 (in green) and NBR2=0.07 (in red).

4.3.3 Surface area coverage by the different composites

For composite B, which only takes into account the NDVI threshold for bare soils, the soil exposure was above 30% for all acquisition dates except for the middle of the growing season (end of May until July, Figure 4.8A). When applying both NDVI and NBR2 thresholds (composite E) the winter months disappeared together with an overall reduction of exposed soil pixels. Composite I based on the combination of the greening-up approach and $NBR2_{0.07}$ threshold allowed for a very limited soil exposure. Only five dates in spring and autumn out of the 36 S-2 images produced more than 10% soil exposure (Figure 4.8A). A link between the weekly rainfall and the decrease in exposed surface when applying the $NBR2_{0.07}$ threshold is observed during winter months (Figure 4.8B). The exposed surface on composite E drops compared to composite B between October 2019 and February 2020. No particular link is observed between weekly precipitation and exposed soil surface on composite E during the months of April, May and June, probably because the surface of the soil dries up quickly in late spring and early summer temperatures. Contrarily, the S-2 overflight of three images from months of July and August (2019-08-24, 2020-07-31, 2020-08-08) took place where no weekly precipitations were measured. Yet, the exposed soil surface on these three images dropped consequently after applying $NBR2_{0.07}$ threshold. This is likely due to the presence of dry residues of cereals on the soil surface. The cumulative percentage of croplands with exposed soils showed that for a two year period, composite B yielded 95% soil exposure, composite E 87%, composite F 88%, and composite I 62% (Figure 4.9). For the greening-up approach, the biggest increase occurred in May and September 2019, which corresponds to the seeding periods of summer and winter crops. Finally, for all pixels included in composite I, the crop type in 2019 was extracted from the dataset of Walloon croplands (Figure 4.10). The results

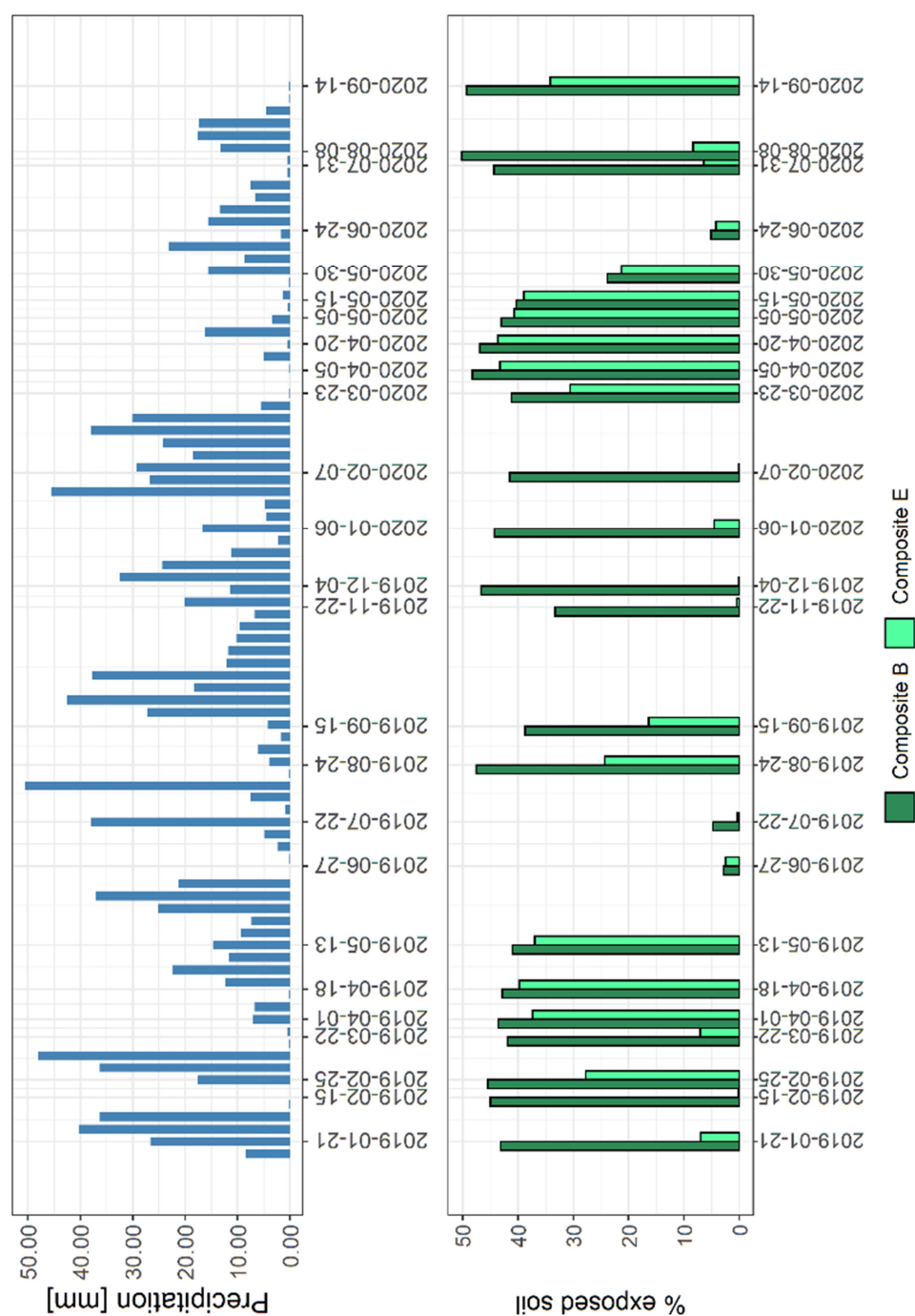
Sentinel-2 exposed soil composite

suggest that for the six main crops, winter cereals and maize are underrepresented in composite I, while peas, sugar beet and potatoes are overrepresented.



(A)

Sentinel-2 exposed soil composite



(B)

Sentinel-2 exposed soil composite

Figure 4.8: Evolution of the percentage of exposed soil on each Sentinel-2 cloud-free image between January 2019 and December 2020 based on the composite criteria selection strategy (A) and the timeline of cumulated weekly precipitation within the area and the percentage of exposed soil on composites B (NDVI only) and E (NDVI and NBR2). For visual reasons, some Sentinel-2 acquisition dates were removed from (B). Source of the weather data: The Royal Meteorological Institute of Belgium.

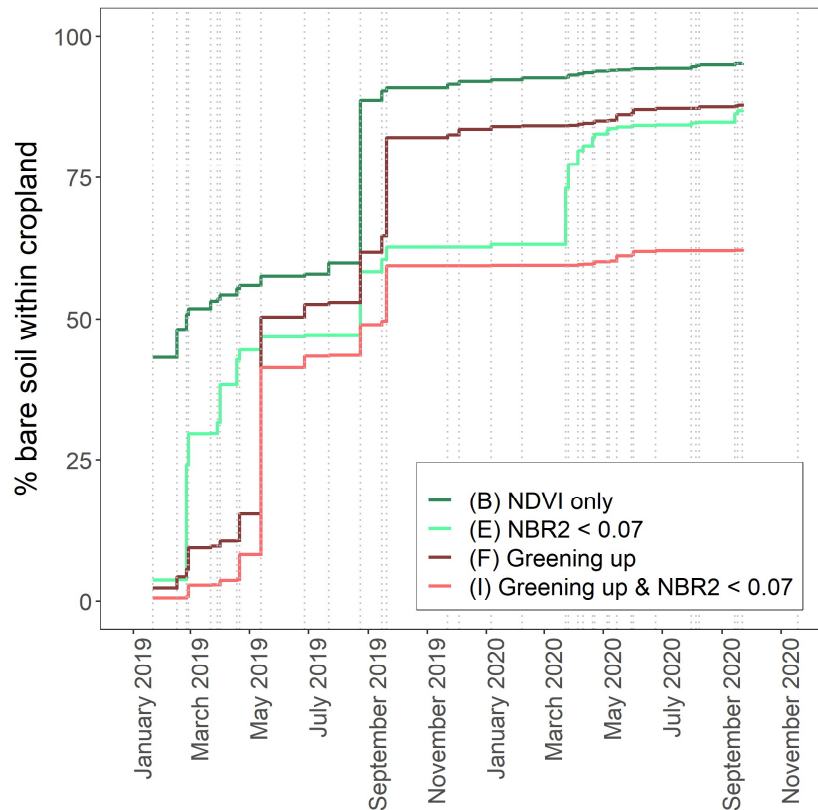


Figure 4.9: Cumulative percentage of exposed croplands extracted from all cloud free S-2 images between January 2019 and December 2020, depending on the composite selection criteria (B, E, F or I). The vertical dashed lines are the S-2 acquisition dates.

Sentinel-2 exposed soil composite

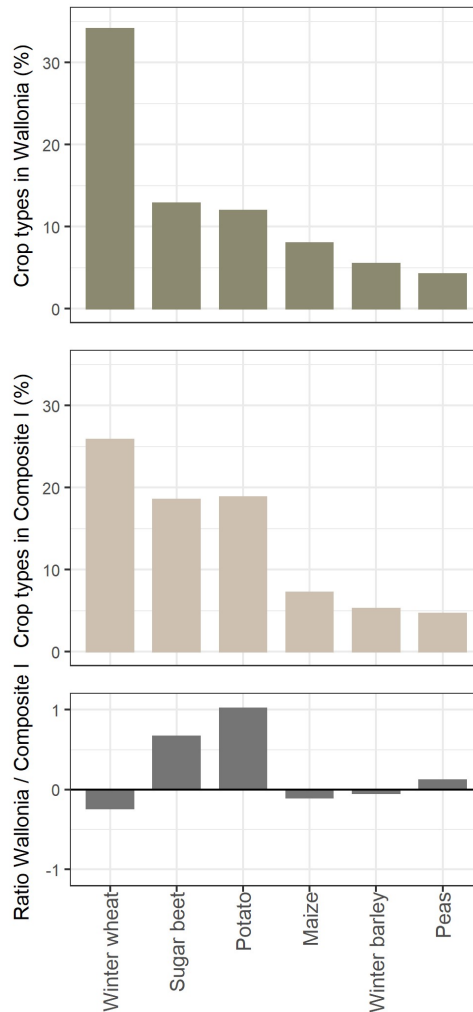


Figure 4.10: *The percentage of surface cover of the main 6 types of crops in the Walloon region (top), the representation of the main 6 types of crops in the Composite I (middle) and the logarithm of the ratio between the two (bottom).*

4.4 DISCUSSION

As several studies have shown (Vaudour et al. 2021; Vaudour et al. 2019b), the SOC prediction model performance from S-2 images relies on the selection of the acquisition date. This selection depends on a number of

factors that influence the state of the soil surface during the overpass (Vaudour et al. 2019b). The factors are mainly related to crop development (e.g. crop and residue cover), weather conditions (e.g. soil moisture content) and agricultural practices (e.g. soil crust and soil roughness).

When we only considered an NDVI threshold to mask vegetation, several single date S-2 images could detect the exposed soil for at least 40% of the cropland surface (Figure 4.8A). Yet, the SOC prediction for none of these single-date images reached a R^2 higher than 0.25, with RMSE that does not drop below 2.50 g C kg⁻¹ (Figure 4.4). If an NBR2_{0.07} threshold was applied, the model performance increased, in some cases up to R^2 of 0.77 and RMSE dropped to 0.5 g C kg⁻¹, but the area that could be mapped dropped to less than 10 % of the cropland (22-03-2019, Figure 4.4 and Figure 4.9). Hence, the choice of acquisition date for achieving a good SOC prediction performance is crucial, while at the same time mosaicking can increase the area covered by the SOC models. Here, we therefore focused on an objective set of criteria for selecting the optimal acquisition dates to be included in an image composite for SOC prediction.

The soil remote sensing community widely uses NDVI thresholds to extract exposed soil in single images (Gomez et al. 2012; Stevens et al. 2010; Vaudour et al. 2016). However, Vaudour et al. (2021) have demonstrated the inadequateness of the NDVI index on its own for creating a temporal mosaic of exposed soil for the purpose of soil property prediction. This is in agreement with our findings. After all, the SOC prediction performance is poor for a composite based on NDVI only (composite B; Table 4.2, Figure 4.5). It is worth inquiring whether creating a soil composite using pixels with the lowest value of NDVI of the time series performs well for SOC prediction. Moreover, SOC prediction performance is not even acceptable for composites using combined NDVI and NBR2 thresholds (composites C to E; Table 4.2, Figure 4.5). This is in contrast to Vaudour et al. (2021) who have obtained acceptable SOC

prediction in the Versailles Plain, France. This is likely caused by their prior removal of images acquired in winter, which was not done here. The sun zenith angle drops below 70° on winter scenes, which hampers the correct estimation of atmospheric parameters used for converting Level-1C to Level-2A product (Vermote et al. 2016). Consequently, the uncertainty of a Level-2A S-2 product is higher for these scenes (Vermote et al. 2016). In addition, winter acquisition dates witness high soil surface moisture, which strongly affects the overall shape of the reflectance spectra of a pixel. This effect is not always filtered by an NBR2 threshold if soils are moist and covered with residues, as NBR2 shows mixed reaction to soils where both crop residues and high soil moisture are combined (see findings in Chapter 3). This is in agreement with Daughtry and Hunt (2008) who stated that remotely sensed estimates of crop residue cover are erratic and unreliable without a robust correction for scene moisture content. Hence, it is difficult to apply a single NBR2 threshold to extract bare soils, and we opted for arbitrary classes of NBR2. So far no conventional threshold for NBR2 has been discussed in the literature: for example Castaldi et al. (2019a) have, by trial and error, tested various NBR2 thresholds to exclude spectra affected by high soil moisture content or crop residues, while Vaudour et al. (2021) have applied NBR2 thresholds corresponding to the 1st quantile, the median and the 3rd quantile of the NBR2 distribution.

We have applied the greening-up method to select the most suitable acquisition date for each pixel. This method allowed narrowing down the number of spectra used for the PLSR model, by pinning down the period during which soils are most likely to be exposed and smooth. The soil pixels selected based on the greening-up criterium are likely to be in seedbed condition i.e. residues have been ploughed in and the soil is smooth after harrowing. The greening-up approach applied on its own (composite F) did not result in a correct SOC prediction either: the prediction performance dropped compared to the composites relying on the NDVI

Sentinel-2 exposed soil composite

and NBR2 indices in synergy or individually (Table 4.2, Figure 4.5). By applying a strict NBR2 threshold, however, the quality of prediction greatly improved (composite I, $R^2 = 0.54 \pm 0.12$, $RPD = 1.68 \pm 0.45$ and $RMSE = 2.09 \pm 0.39 \text{ g C kg}^{-1}$, Table 4.2). This is due to the fact that during the greening-up period, soils are without residues. Under such conditions the NBR2 index appears to be reliable for masking moist soils. Hence, the combination of greening-up and NBR2 extracts smooth, bare soils that are dry. Further research is needed to test the robustness of the NBR2 to mask moist pixels for these soils without residues.

The SOC pixels predicted using composite I (the greening-up method combined with a strict NBR2 index) covered more than 62% of the arable cropland for images acquired during two years. This exceeds at least three-fold the amount of exposed soil pixels of the single date S-2 images which allowed for a similar SOC prediction accuracy, i.e. $R^2 > 0.5$ and $RMSE < 2.00 \text{ C kg}^{-1}$ (21-01-2019, 22-03-2019, 01-06-2020, 31-07-2020, 05-08-2020 and 08-08-2020, Figure 4.4). The months of April, May, August and September accounted in our case for the biggest increase in exposed croplands. This is in agreement with the crop calendar of the Walloon region, i.e. potatoes, sugar beet and maize are sown in April/May, and winter cereals are sown in September.

Rogge et al. (2018) developed an automated process to overcome the issue of limited soil exposure in satellite images, the Soil Composite Mapping Processor (SCMaP). The output generated by SCSMaP is the average reflectance per pixel of each spectral band over a variable time period. Such averaging allows for the reduction of variability in the exposed soils, caused by factors such as crop residue cover, moisture and roughness (Rogge et al. 2018). They used five-year time periods to create exposed soil composites with sufficient soil cover on the one hand, and comparable data products from 1984 to 2014 on the other (Rogge et al. 2018). The longer time period was necessary

to account for the lower repetition rate of the Landsat sensors (16 days), which can now be reduced to two years for Sentinel-2 (5 days when both S-2A and S-2B are used). For the same area, van Wesemael et al. (2019) have shown that the change in SOC contents of croplands was negligible at on average 0.27 g C kg^{-1} over a ten year period. SCMaP is also a flexible tool to produce season-specific composites, and its product has been used locally for SOC prediction by Žížala et al. (2019). Vaudour et al. (2019b) suggested the inclusion of only specific periods (i.e. spring versus autumn), as they provided the best results in the Versailles Plain. Yet, at larger scales, the regional phenology varies and such selection of single suitable sensing period might constrain the results. We, on the other hand, proposed a method where a limited amount of scenes is selected based on the greening-up period, and only such scenes were included in the final composite. We applied a simple algorithm relying on binarized NDVI information, which diminished the computational time. However, many simplifications were made, and our approach does not reach the complexity of for example the TIMESAT algorithm, which defines key phenology dates and retrieves a set of phenology metrics (Tan et al. 2011). Additionally, the use of updated crop calendars, if they were available for the study area, would reduce the amount of calculations, as it would pin down the cropping period. Nevertheless, the greening-up method can probably be applied in most regions of the world. We believe that the key to success lies in the combination of the SCMaP multiple year approach which stabilizes the signal, with the greening-up approach that narrows down the number of satellite images, independently of the region. Additionally, the SCMaP derives thresholds for spectral indices by using temporal spectral data and existing land cover data (Rogge et al. 2018). This allows for automatic threshold selection for various regions of the world, thus bypassing the need for manual selection of NDVI and NBR2 thresholds, as was done here.

4.5 CONCLUSIONS

Several authors have used composite images to increase cropland area for which SOC content can be predicted. The surface conditions have, however, hindered the accuracy of the SOC prediction models. Hence, spectral indices are being used by many authors to discriminate between soils in suitable and unsuitable conditions. However, the amount of available spectral indices on the multispectral Sentinel-2 is limited, and the width of the spectral bands does not allow for a straightforward detection of disturbing effects such as crop residues, soil moisture and soil roughness. To select the most appropriate pixels to be included in a composite image for SOC prediction, we have explored the potential of pinning down the right acquisition date for each pixel based on the crop calendar. We defined as greening-up the instant for which the crop has been sown but has not yet emerged. This means that an eventual crust and crop residues have been ploughed in and soils are in seedbed condition (i.e. smooth). This is the closest we are able to get to the pure soil signal of the surface spectrum. Once the crop residues were removed by selecting the greening-up moment, we applied the NBR2 index in order to remove pixels with high moisture contents. This greening-up-NBR2 combination applied as a threshold for a two year series of S2 images provided a SOC prediction model with a fairly good performance ($R^2 = 0.54 \pm 0.12$, $RPD = 1.68 \pm 0.45$ and $RMSE = 2.09 \pm 0.39 \text{ g C kg}^{-1}$), and covered 62% of the cropland. Overall, the greening-up-NBR2_{0.07} synergy is a relatively simple (based on NDVI and NBR2), automated and objective method for accomplishing a trade-off between model performance and surface cover.

CHAPTER 5. IMPROVING SOC PREDICTIONS FROM A SENTINEL-2 COMPOSITE BY ASSESSING SURFACE CONDITIONS AND UNCERTAINTIES³

OUTLINE

In the previous chapters, we have demonstrated the importance of selecting the right soil surface conditions for SOC prediction (Chapter 3), and the advantage of using composite imagery to stabilize the soil signal and increase the mappable area (Chapter 4). In this chapter we aim to combine these two main findings, and define the most appropriate methodology for creating the most suitable exposed soil composites for SOC mapping from S-2. For this, in-situ field observations of the soil surface conditions of croplands in Belgium were acquired, and were linked to their spectral signature extracted from S-2 imagery. These observations allow to determine NDVI and NBR2 thresholds which need to be used to obtain soil composite including only pure soil spectra. This composite is then used to create SOC prediction maps.

Additionally, McBratney et al. (2003) have stated that digital maps of soil properties should be accompanied by a measure of their associated spatial uncertainty. This uncertainty of prediction must be assessed to characterize the quality of the prediction maps and to define which uncertainty limits are tolerated (Gomez et al. 2019; McBratney et al. 2003). Compared to the common model performance indicators such as R^2 , RMSE or RPD which

³ The content of this chapter was published in Dvorakova, K., Heiden, U., Pepers, K., Staats, G., van Os, G., & van Wesemael, B. (2022). Improving soil organic carbon predictions from a Sentinel-2 soil composite by assessing surface conditions and uncertainties. *Geoderma*, 116128

*Improving SOC predictions from a Sentinel-2 composite by
assessing surface conditions and uncertainties*

are calculated only from points for which the reference values are known, the uncertainty maps can be calculated for all new predictions. Until this day, there remains a scarcity of uncertainty maps for SOC predictions from remote sensing. Hence, Chapter 5 is focused on uncertainty assessment for SOC prediction maps from S-2 exposed soil composite. One source of uncertainty is assessed: model uncertainties due to the training data using a bootstrapping procedure, as that is the most commonly used way to estimate uncertainty in soil property predictions (Brodský et al. 2013; Gomez et al. 2019; Gomez et al. 2015; Viscarra Rossel and Hicks 2015).

5.1 INTRODUCTION

The previous chapter has discussed the effects of using a spectral index for unpure pixel removal from exposed soil composite on SOC prediction. The index thresholds in the mentioned studies (Diek et al. 2017b, Demattê et al. 2018, Gallo et al. 2018, Rogge et al. 2018, Loiseau et al. 2019, Vaudour et al. 2021) including Chapters 3 and 4 of this thesis were chosen on trial and error basis. The extent to which these index thresholds distinguish between different soil surface conditions is rarely reported and may also be specific for pedoclimatic zones. Hence, the first goal of this chapter is to use field observations to determine observation-based index thresholds to eliminate pixels with disturbing effects.

McBratney et al. (2003) have stated that digital maps of soil properties should be accompanied by a spatial measure of their associated uncertainty. This uncertainty of prediction must be assessed to characterize the quality of the prediction maps and these limits allow the user to define whether the product is suitable for the intended use (Gomez et al. 2019; McBratney et al. 2003). Compared to the common model performance indicators such as MEC, RMSE, RPD or RPIQ which are calculated only from points

Improving SOC predictions from a Sentinel-2 composite by assessing surface conditions and uncertainties

for which the reference values are known, the uncertainty maps can be calculated for all new predictions. One of the rare examples of uncertainty quantification for soil prediction from imaging spectroscopy is provided by Gomez et al. (2015). They analyzed the uncertainties that affect clay content mapping from VNIR/SWIR airborne data. Brodský et al. (2013) have evaluated the spatial uncertainty of the SOC prediction maps acquired by means of field spectroscopy covering a single cropland field in the Czech Republic, and Safanelli et al. (2020) provided uncertainty maps for EU Landsat derived soil maps of clay, CaCO_3 and SOC.

In response to the scarcity of SOC maps accompanied by the uncertainty of prediction, this chapter aims to predict SOC from an S-2 exposed composite and quantify the uncertainty for the croplands in parts of Belgium and The Netherlands. The first part of this chapter consists of gathering in-situ field observations of soil surface conditions of croplands (notably crop residues, soil moisture and soil crusts), and linking them to remote sensing information, more specifically the NBR2 index. Once a NBR2 threshold based on field observations is found that allows eliminating soils in unsuitable conditions for SOC prediction from remote sensing, the exposed soil composite is created using this threshold. The second part of this study focuses on uncertainty assessment for SOC prediction maps from an S-2 exposed soil composite. Here we use bootstrapping to vary the calibration data set and quantify the effects on SOC prediction. Given the large storage and high computing power needed for the creation of exposed soil composite, Google Earth Engine cloud computing platform (Gorelick et al. 2017) is employed for processing bare soil surface spectra using S-2 multi-temporal data. The composite is used to predict SOC over large areas: 16 900 km^2 in southern Belgium, and 6 350 km^2 in the Dutch polders. These zones were selected because of their large cropland extent (5370 km^2).

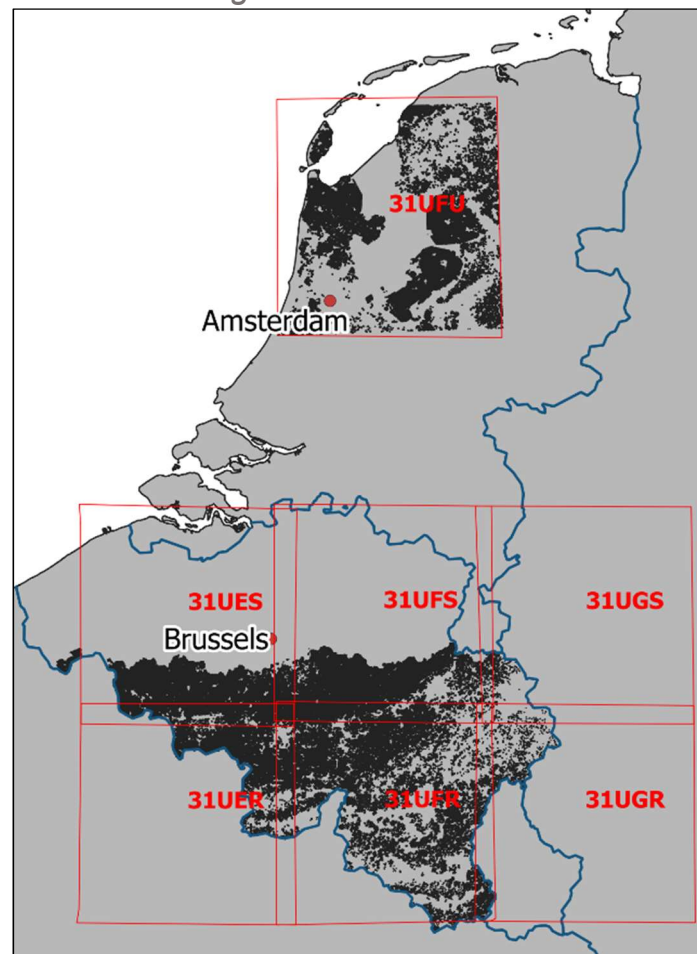
5.2 MATERIALS AND METHODS

5.2.1 Study site

The study was conducted in Wallonia, southern Belgium and in part of Noord-Holland and Flevoland in the Netherlands (Figure 5.1). The study area in Wallonia covers 16 900 km², and is described in section 2.5.2.

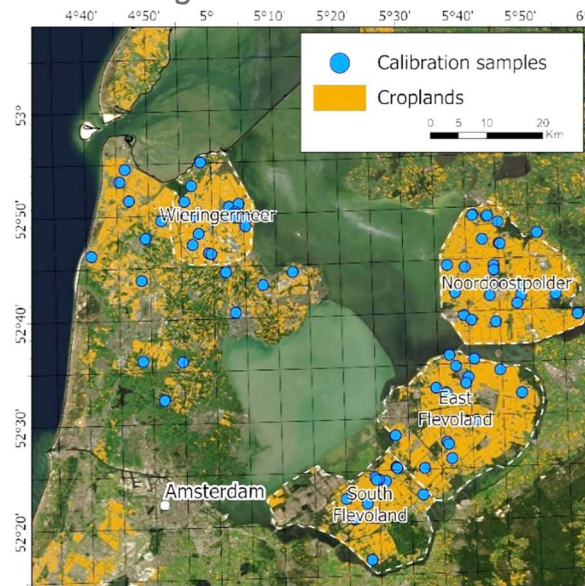
The study area in the Netherlands contains four polders, which were reclaimed from the IJsselmeer during the 20th century (Figure 5.1B) (Waterman et al. 1998). The oldest polder Wieringermeer (drained in 1930) covers 200 km² and is part of the province Noord-Holland. The Noordoostpolder was drained in 1942 and spreads across 480 km². The Flevoland polder was reclaimed in two parts: East Flevoland drained in 1957 (540 km²) and South Flevoland drained in 1968 (430 km²) (Waterman et al. 1998). The soils are calcareous and relatively young, with predominantly loamy soils with clayey intrusions (Fluvisols and Gleysols, WRB (2014)). The agriculture is intensive, with maize, winter wheat and potatoes being the dominant crops. As both the Dutch and Belgian study areas are dominated by conventional agriculture, soil properties are uniform in the top 0-20 cm due to repeated tillage (Meersmans et al. 2009b). Merging these two regions together allows for a higher range of SOC values, which increases the chances of a well performing SOC prediction model.

*Improving SOC predictions from a Sentinel-2 composite by
assessing surface conditions and uncertainties*

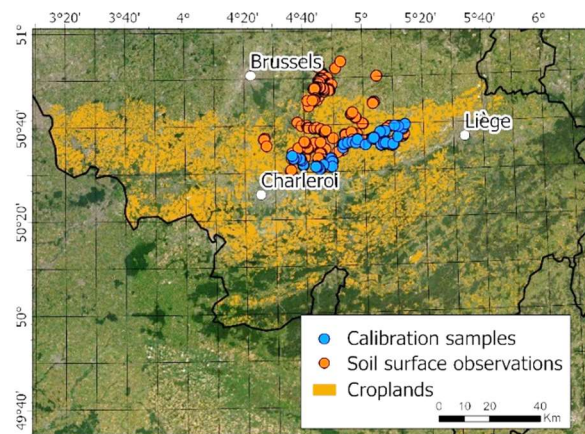


(A)

Improving SOC predictions from a Sentinel-2 composite by assessing surface conditions and uncertainties



(B)



(C)

Figure 5.1: (A) Location of the croplands (in black) and the Sentinel 2 tiles (in red) in Belgium and the Netherlands. Zoom on the two study areas: (B) the polders in The Netherlands and (C) southern Belgium. In red are the 303 in-situ observations of soil surface conditions and in blue the 124 calibration samples. For each blue point in the Belgian loam belt, soil surface observation was made. The 34,385 REQUASUD validation samples are not shown, as they are uniformly distributed over the Walloon region.

5.2.2 Field data

A total of 303 observations of the soil surface were made in the Belgian loam belt region (red points on Figure 5.1C). The data were collected on nine occasions from October 2019 to April 2021 (Table 5.1). The locations were chosen at least 20 m from the field border in order to avoid mixed pixels. For each field observation, an RGB geo-referenced (7-8 m precision) was taken with a smartphone. For each observation we assigned a yes/no variable according to the state of the surface conditions (i.e. seedbed, crop residues, moist soils, growing crops and soil crust). The soil was categorized as moist if puddles were visible or if a color difference could be attributed to partial drying of the soil surface. Ultimately, observations with mixed soil surface conditions (e.g. presence of vegetation on wet soil, etc.) were discarded. At some of the locations, if the conditions allowed it (field was not freshly seeded or vegetation has not developed yet), soil samples were taken on March 2021, avoiding field edges. In total 51 pseudo-random (given site availability) surface soil samples (0-10cm) were collected (Figure 5.1C, referred to as the Belgium calibration dataset). Each sample consists of five sub-samples collected within a circle of 5 m radius centered on the geographical position of a sampling plot, which was recorded by a Garmin GPS with 3 m precision. The sub-samples were then thoroughly mixed and stored in a plastic bag.

Additionally, 73 geo-located soil samples (referred to as Dutch calibration dataset) were collected in June 2021 on the S-2 tile T31UFU (Figure 5.1B). These samples were selected so that (1) they were located in croplands and (2) they covered the principal component space computed from the spectra on a S-2 T31UFU image acquired on 05-04-2020. This image was selected because of the large extent of exposed soils, and the dry conditions preceding the acquisition date. The first two principal components characterizing 70% of the original S-2 image were retained

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to describe the spatial variability, and 100 locations were selected for sampling. Given the non-accessibility of some of the locations, 73 out of the 100 locations were sampled. In total 124 samples were available for calibration in Belgium and The Netherlands. The reason for joining these datasets was to increase the SOC variability in the calibration dataset.

The model predictions were validated on an external and independent dataset. The results from routine analyses for fertilizer advice are available in a database of the REQUASUD network since 2005 (<https://www.requasud.be/>, accessed date: 30 November 2021). The soil data refer to composite samples covering an entire field (or a soil series within a field). A total of 34,385 cropland fields were sampled from 2017 until 2021 (referred to as the REQUASUD independent validation dataset).

5.2.3 Laboratory analyses

All samples (i.e. the Belgium and the Dutch calibration datasets) were air-dried, gently crushed and passed through a 2 mm sieve. SOC was analyzed by dry combustion, using a VarioMax CN Analyzer (Elementar Analysensysteme GmbH, Hanau, Germany), as detailed in Shi et al. (2020b). For samples showing reaction with 10% HCl (1 out of the 51 samples from the Belgian calibration dataset and 62 out of the 73 samples from the Dutch calibration dataset), carbonate content was measured using a modified pressure-calimeter method (Sherrod et al. 2002). Then, SOC was obtained by subtracting the inorganic carbon from the total carbon content. The SOC content of the composite samples of the REQUASUD independent validation dataset is measured via sulfochromic oxidation (ISO 14235) and dry combustion (ISO 10694) (Genot et al. 2012).

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To evaluate the general accuracy of the prediction, the difference for all samples between predicted (by remote sensing) and measured (laboratory) SOC contents (i.e. the residuals) of the external independent dataset was calculated (Equation 5.1).

$$Residuals = SOC_{measured} - SOC_{predicted} \quad (\text{Equation 5.1})$$

5.2.4 Remote sensing data

Remote sensing data were obtained using the Multi-Spectral Instrument (MSI) on board of the Sentinel 2-A (S-2A) and S-2B platforms (see section 2.5.1). S-2 imagery was obtained as Level-2A product; i.e. geometrically, radiometrically and atmospherically corrected using sen2cor, in the Google Earth Engine (GEE) environment (COPERNICUS/S2_SR). The sen2cor correction here is chosen, rather than the MAJA correction used in Chapter 4 and the SNAP correction used in Chapter 3, because it is easily available in GEE. Seven S-2 tiles 31UFU, 31UES, 31UER, 31UFS, 31UFR, 31UGS and 31UGR were used. A cloud mask precomputed with the *s2cloudless* Python package, and available as GEE COPERNICUS/S2_CLOUD_PROBABILITY product, was used to remove pixels affected by clouds (pixels with 'probability' < 30 were kept). Cloud shadows were not treated. We used nine bands (B2, B3, B4, B5, B6, B7, B8, B11 and B12) resampled to 20 m resolution. The spatial resolution of S-2 pixels used in this chapter differs from Chapters 3 and 4 (10m), for the only reason of the reduction of processing time. The images were masked using the Walloon cropland map extracted from the Land Parcel Information system for Wallonia in 2019 (<http://geoportail.wallonie.be>, accessed date: 28 January 2021) and the Dutch cropland map 2017 from the Ministry of Economic Affairs and Climate (<https://data.overheid.nl>, accessed date: 5 July 2021).

5.2.4.1 Sentinel-2 single date imagery

The S-2 spectrum was extracted for each of the 242 geolocated field observations to link these with S-2 imagery. For each field observation, the closest S-2 acquisition date was selected (Table 5.1). The time difference in ground campaign and image acquisition was in the majority of cases not more than two days (Table 5.1). However, at three occasions the S-2 image was acquired more than three days after the ground campaign. It was ensured that the weather conditions between the ground campaign and image acquisition remained similar. Fields that were in seedbed condition during the ground campaign and for which the image was acquired more than two days ahead of time (this is the case for the October field campaign) were not included in the sample to minimize the chance of false observations, as it is not possible to know how long ago the field was ploughed.

The normalized reflectance was derived to highlight the spectral shape and reduce the amplitude of variation of the spectra (Rogge et al. 2018):

$$Mean\ reflectance = \frac{SUM_{b \in [1, Nb]} reflectance_b}{Nb}$$

(Equation 5.2)

$$Normalized\ reflectance_b = \frac{reflectance_b}{Mean\ reflectance}$$

(Equation 5.3)

where Nb is the total number of bands, and $b \in [1, Nb]$ is the band number, and varies from 1 to 9 (B2, B3, B4, B5, B6, B7, B8, B11 and B12). The normalization was used for the purpose of albedo difference removal.

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The NBR2 spectral index was calculated for the 242 S-2 spectra (Equation 2.10). It was then compared amongst the five soil surface categories, with the aim to obtain an $NBR2_{threshold}$ value that separates moist soils and soils with crop residues from the other categories.

Table 5.1: *The acquisition date of the geolocated field observations, versus the acquisition date of the Sentinel-2 (S-2) imagery.*

Number of field observations	Field date	Closest S-2 acquisition date
24	18 October 2019	13 October 2019
12	27 March 2020	26 March 2021
16	1 April 2020	
41	2 April 2020	5 April 2020
27	4 April 2020	
107	31 March 2021	31 March 2021
37	1 April 2021	
22	26 April 2021	25 April 2021
17	29 April 2021	27 April 2021

5.2.4.2 Sentinel-2 multi-temporal series

We used Sentinel-2 spectra acquired during the spring months from 2016 to 2021 (March, April and May) to build the exposed soil composite in GEE environment by a pixel based multi-temporal analysis. The compositing refers to the process of combining spatially overlapping images into a single image based on an aggregation function, in this case the mean. The mean of the selected exposed soil pixels was chosen because it is the most common approach

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in soil compositing for the moment (Diek et al. 2016; Rogge et al. 2018; Vaudour et al. 2021). In total, 158 images per S-2 tile were used. We focused on the spring months because this is the period in temperate cropping systems when the maximum extent of bare soil occurs during preparation for and sowing of the summer crops (e.g. sugar beet, potato, maize). Moreover, the soil surface dries out quickly during sunny conditions that are required for a cloud free S2 image and the sun zenith angle is already high (avoiding the winter months when sun zenith angle drops below 70°). The low sun zenith angle hampers the correct estimation of atmospheric parameters used for converting Level-1C to Level-2A product (Vermote et al. 2016). Then the spectra were normalized (Equation 5.3), and the $NBR2_{\text{threshold}}$ defined from the field observations is applied to mask out moist soils and crop residues. Additionally, the NDVI (Rouse et al. 1974) was calculated (Equation 2.7). NDVI threshold of 0.25 was retained from Chapter 4 to mask green vegetation. For all images, pixels with NDVI values above 0.25 were considered as pixels containing green vegetation.

Overall, only the pixels which comply with the following conditions were kept: no clouds, $\in$ cropland, $NDVI < 0.25$, $NBR2 < NBR2_{\text{threshold}}$. The $NBR2_{\text{threshold}}$ used was found following the methodology in section 5.2.4.1. Since an image collection from spring months 2016-2021 was used (in total 158 images per tile), it is very likely that several dates comply with the above-mentioned conditions for a pixel, i.e. the number of scenes per pixel > 1 . Therefore, we computed the mean reflectance value for each band per pixel. This mean value represents the final exposed soil composite, which was used for SOC prediction. Note that as cloud shadows have not been removed, they might affect the composite. For further analysis, the number of scenes contributing to the mean spectrum of each pixel was calculated and stored in a database.

5.2.4.3 SOC prediction models

Exposed mean soil composite reflectance values (section 5.2.4.2) were regressed against topsoil SOC contents from the corresponding pixels in the calibration dataset (n=124) in order to calibrate a SOC model. The partial least squares regression (PLSR) model was then chosen to construct the SOC prediction models (section 2.3.4.1). The maximum number of LV's was set at five in order to avoid over-fitting the model. The Variance Importance Projection (VIP) index was calculated in order to detect the main spectral regions involved in the SOC prediction. Spectral bands with VIP values greater than one were considered important in the PLSR model.

The quality of model fit was assessed using the following parameters: Model Efficiency Coefficient (MEC) which is the equivalent of the R-square of predicted and observed values computed against the 1:1 line (Equation 5.4), Root Mean Square Error (RMSE) (Equation 2.5), Ratio of Performance to Deviation (RPD) (Equation 2.6) and Ratio of Performance to Interquartile Range (RPIQ) (Equation 5.5) of ten-fold cross-validation:

$$MEC = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (\text{Equation 5.4})$$

$$RPIQ = \frac{IQ}{RMSE} \quad (\text{Equation 5.5})$$

where $\hat{y}$ = predicted value, $\bar{y}$ = mean observed value, y = observed values, n = number of samples with $i = 1, 2, \dots, n$, and IQ the interquartile range (quartiles 0.25 and 0.75) of the observed values. According to Bellon-Maurel and McBratney (2011), RPIQ index presents a more realistic evaluation of a model rather than RPD, when working with non-normal data .

Additionally, each set of calibration samples was subject to bootstrapping to stabilize the prediction model performance,

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and to calculate the variance of prediction, which is an input in the measure of uncertainty (Malone et al. 2011). Bootstrapping consists of repeatedly calculating a given statistic from a series of subsamples obtained by randomly resampling with replacement an initial dataset (Efron and Tibshirani 1993). Hence, 100 PLSR models were created (100 bootstraps), each with a different calibration dataset of 124 samples, drawn with replacement from the original sample that has the same sample size. These models were applied to the exposed soil composite, resulting in 100 SOC prediction maps of the area.

5.2.5 SOC maps and their uncertainty

The 100 SOC prediction maps were averaged at each point in space in order to obtain one prediction value per pixel (Figure 5.2), while the variance of the 100 predictions as well as the mean squared error (MSE) estimated from the cross-validation were used to quantify uncertainty (Malone et al. 2016). An overall prediction variance at each pixel is the sum of the random error component (MSE) and the bootstrap prediction variance as follows ((Equation 5.6), Malone et al. (2016)):

$$VAR_{all} = VAR_{boot} + MSE_{vali} \quad (\text{Equation 5.6})$$

where VAR_{all} is the overall variance i.e. the sum of the variance of the 100 bootstrap predictions and MSE_{vali} the mean square error estimated by validation. To derive the 90% prediction interval, the square root of the variance estimate is multiplied by the z value that corresponds to 90% probability ($z=1.64$), to calculate the Standard Error (SE, (Equation 5.7)):

$$SE = \sqrt{VAR_{all}} \times z \quad (\text{Equation 5.7})$$

The Upper (Equation 5.8) and Lower (Equation 5.9) Prediction Limits (UPL and LPL) are then calculated:

$$UPL = MEAN_{boot} + SE \quad (\text{Equation 5.8})$$

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$$LPL = MEAN_{boot} - SE \quad (\text{Equation 5.9})$$

Where $MEAN_{boot}$ is the mean bootstrap prediction. The Prediction Interval Range (PIR) is then the difference between the UPL and LPL (Equation 5.10):

$$PIR = UPL - LPL \quad (\text{Equation 5.10})$$

Here, we express the model output uncertainties as the PIR (Malone et al. 2011). To assess whether a link exists between the number of scenes per pixel and the uncertainty, 5000 points were randomly selected within the croplands of the loam belt (2500 points) and the croplands of the polders of Flevoland and Wieringermeer in the Netherlands (2500 points). For each of these points, new composites were created from the S-2 time series (section 5.2.4.2), where the number of scenes per pixel included in the calculation of the composite varied from 1 to N. The composite spectra were calculated as follows: for each of the 5000 points of $Dataset_n$, randomly extract $n \in [1, N]$ spectra from the Sentinel-2 time series, and calculate the mean of the selected spectra if $n > 1$. Hence, n represents the number of scenes per point (Figure A.5.1). For example, the points in $Dataset_4$ contain the mean of four spectra randomly selected from the Sentinel-2 time series for each of the 5000 points. The PLSR model with bootstrapping as described above was then applied to the 5000 points of each dataset, creating a database of SOC predictions with dimensions $N \times 5000 \times \text{bootstraps}$. Given the large computational load of this procedure, the number of bootstraps was set to 50 and N was set to 24. To guarantee that the datasets were balanced, it was ensured that each of the 5000 randomly extracted pixels appeared on at least 24 scenes. Finally, the uncertainty is calculated for each point of each $Dataset_n$. Based on this, the minimal number of scenes per pixel F_{min} which allows to minimize the uncertainty of SOC predictions is found. All pixels for which the number of scenes on the exposed soil composite $< F_{min}$ are then eliminated. Since SOC predictions per pixel might

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suffer from noise, due to for example mixed pixels, the SOC prediction information is aggregated per field. This also allows validating the results against the independent REQUASUD dataset which provides SOC content of composite samples collected in 34,385 fields. After eliminating pixels for which the number of scenes $< F_{\min}$, the 100 SOC prediction maps are each averaged per field, providing 100 mean values per field. Fields which contain less than 10 pixels were eliminated to avoid errors due to mixed pixels in such very small fields.

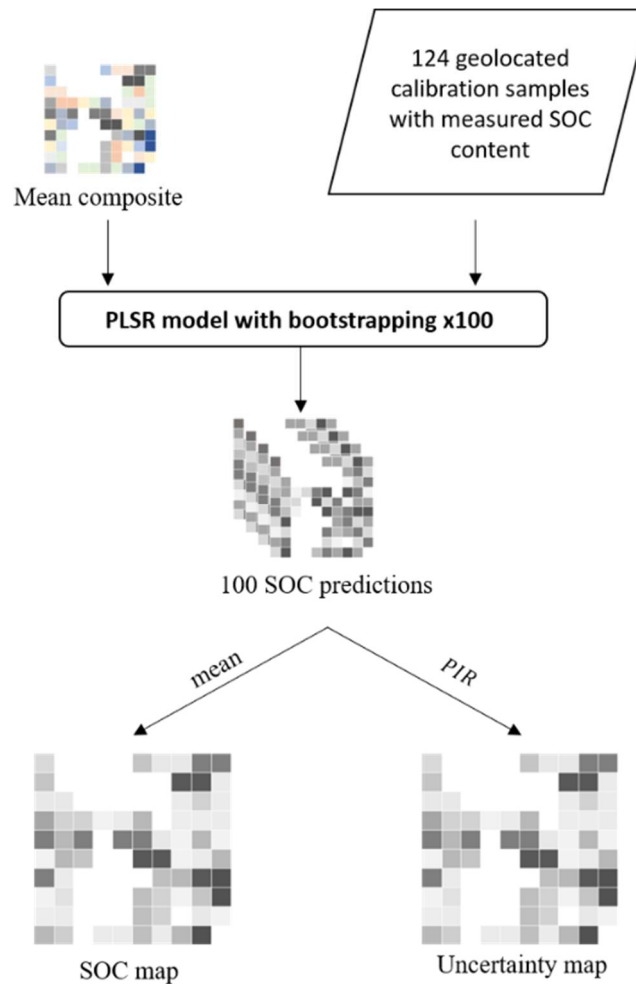


Figure 5.2: General flowchart for the SOC modelling from the exposed soil composite.

5.3 RESULTS AND DISCUSSION

5.3.1 In-situ observations of soil conditions

242 observations of soil surface out of the 303 presented only one time of soil surface disturbance: (a) seedbed (n=76), (b) crop residues (n=38), (c) moist soils (n=13), (d) growing crops (n=10), and (e) soil crust (n=114). The 242 extracted S-2 spectra were classified into five classes based on the observations of the surface conditions (Figure 5.3), and the spectra were normalized (Equation 5.3) and averaged per category (Figure 5.4). The spectrum of a soil in seedbed condition is the desirable shape for soil property prediction from remote sensing. The spectrum of vegetation shows recognizable features in the visible and infra-red region, with high absorption in B4 due to photosynthetic activities and high reflectance in B8 due to leaf structure (spongy mesophylls; Figure 5.4) (Rouse et al. 1974). The NDVI was designed to quantify this increase in reflectance and spectra affected by vegetation can be differentiated from exposed soils with an NDVI threshold. The spectrum of a soil crust has an overall higher albedo than a spectrum of a soil in seedbed condition, but has a similar shape (Figure 5.5A). According to the literature, the effects of crusts on reflectance are mainly translated in a change of albedo, with absorption features varying slightly at 1450 nm and 1900 nm (Ben-Dor et al. 2003). Since these spectral regions are not corresponding to any of the S-2 MSI band, we hypothesize that structural crusts in the loam belt region in Belgium only affect the soil albedo, and the albedo shift can be corrected for by spectral normalization (Figure 5.5B). This hypothesis still has to be studied in other geographic conditions. For example, the colonization of physical soil crusts by algae or lichens in semi-arid and arid regions induces a large spectral variability at 550, 680 and 750 nm, due to chlorophyll absorption (Chamizo et al. 2012). This chlorophyll absorption feature might be observable on S-2

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spectra, and a simple spectral normalization will not be enough to mask such biological soil crusts.

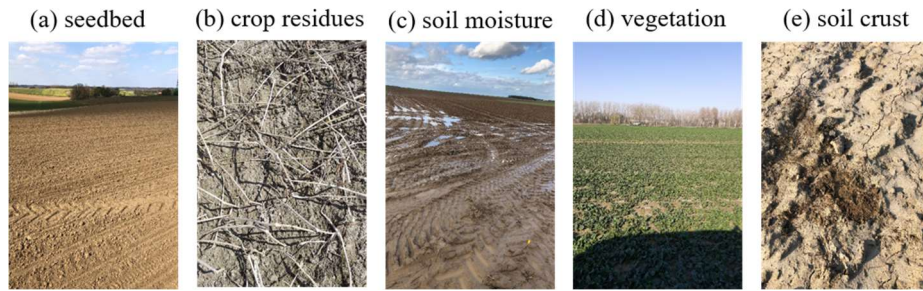


Figure 5.3: *Examples of the five categories of soil surface conditions in Belgian croplands.*

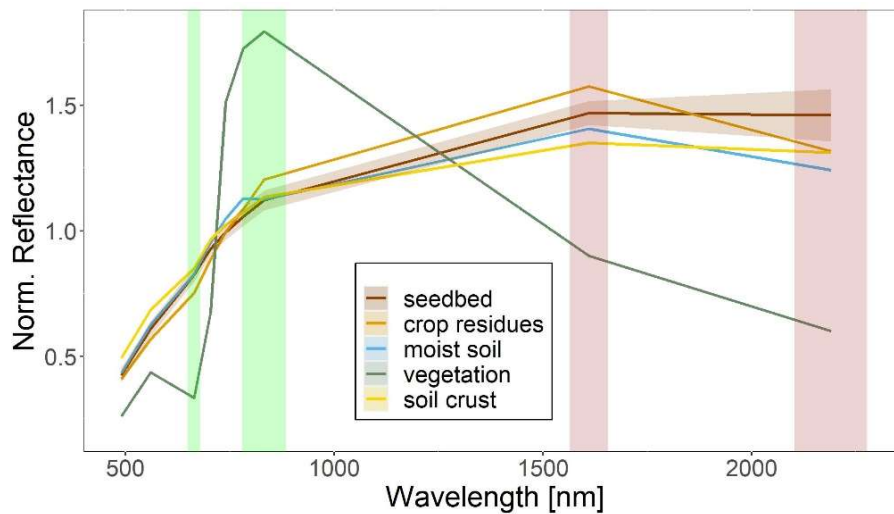


Figure 5.4: *Mean S-2 spectra for each category of the five soil surface conditions in the Belgian loam-belt. For the sake of clarity of the figure, the standard deviation of the spectra is only provided for the spectrum of a soil in seedbed conditions, i.e. the optimal condition for soil mapping from remote sensing imagery. The green vertical bands indicate the S-2 B4 and B8 used to calculate NDVI and the brown vertical bands are S-2 B11 and B12 used to calculate NBR2.*

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Additionally, soil albedo is not only affected by soil crusts. In fact, Muller and Décamps (2001) observed strong impact of soil moisture on soil albedo, and Franceschini et al. (2015) observed that soil spectral albedo decreases when SOC and clay content increases. Therefore, by normalizing the spectra, the albedo effect caused by soil crust, soil moisture, but also by SOC are eliminated. This might lead to a reduction in the predictive power of the SOC models which use normalized spectra as input.

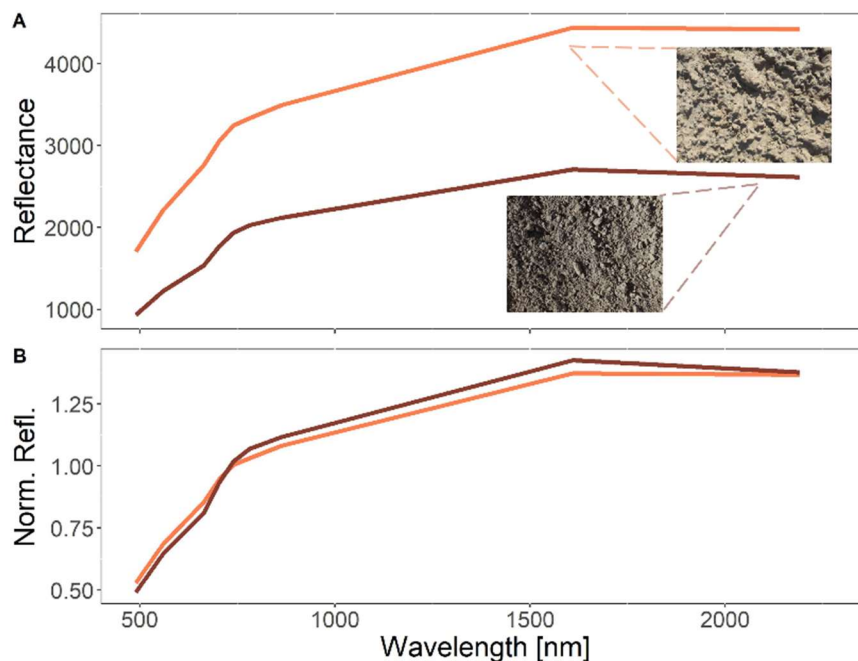


Figure 5.5: (A) S-2 spectra for the same location extracted at two dates: 26 March 2020 (orange line) when soil crust was present, and 28 March 2020 (brown line) when the soil was in seedbed condition. (B) The same S-2 spectra but normalized.

Finally, the spectra of moist soils and soils with crop residues (i.e. non-photosynthetically active vegetation) show a higher absorption in B12. For crop residues this absorption feature is due to the structural compounds of cellulose, hemicellulose and lignin found in dry residues at 2100 nm (Daughtry et al. 1996). The higher absorbance in

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B12 for moist soils is a result of the strong absorption band between 1750-2000 nm due to water, that also impacts the adjacent wavelength regions covered by B11 and B12. Hence, the NBR2 index, which quantifies the difference between B11 and B12 shows a stronger response to spectra affected by soil moisture and crop residues, rather than to spectra of soil crusts and of soils in seedbed conditions (Figure 5.6). Given the high absorption of photosynthetically active vegetation in B12 due to high water content, the NBR2 index is also important for vegetation. ANOVA analysis of soils with crust and in seedbed conditions against moist soils, vegetation and crop residues showed a significant difference in NBR2 (at $\alpha=0.10$ significance level). An NBR2 threshold of 0.05 was found to be able to differentiate soils with crust and in seedbed conditions from moist soils, vegetation, and crop residues (Figure 5.6).

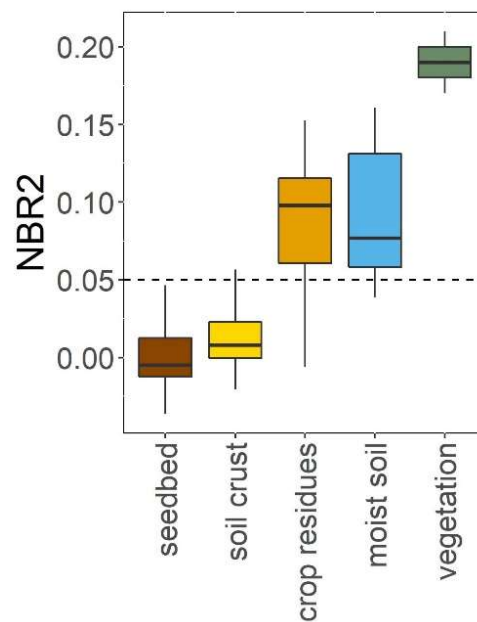


Figure 5.6: NBR2 for the 242 in-situ soil surface observations in the Loam Belt region in Belgium, categorized into five classes. An NBR2=0.05 threshold can separate vegetation, crop residues and moist soils from soils with crusts and in seedbed condition.

5.3.2 Exposed soil composite comparison with in-situ soil observations

An exposed soil composite image for the areas of interest (Figure 5.1) was built from the S-2 image collection. The greening-up method found in Chapter 4 was not used here, because of the large computational power needed to process S-2 tiles covering Belgium and the Netherlands. The pixels which complied with the following conditions were kept: no clouds, $\in$ cropland, $\text{NDVI} < 0.25$, $\text{NBR2} < 0.05$. For comparison with the soil surface categories, the composite spectra for 242 in-situ observation locations were averaged per class. The mean normalized spectrum showed a close resemblance to a spectrum of a soil in seedbed conditions and soil crusts (Figure 5.7). The widespread occurrence of soil crusts during the spring months is reflected in the spectra of the composite, although the difference to the spectra of the seedbeds is minimal. Overall, the combination of $\text{NBR2} < 0.05$ threshold and spectral normalization increases the likelihood of including only spectra in suitable conditions in the exposed soil composite.

An important step in the methodology was the definition of thresholds to discriminate soils from other targets (vegetation, wet soils and crop residues). These thresholds are site specific, and no rule of thumb exists to adjust them according to regional or local spectral patterns (Demattê et al. 2020). The common NDVI thresholds used in the literature for vegetation masking are 0.20 (Gholizadeh et al. 2018; Gomez et al. 2016; Lagacherie et al. 2019), 0.25 (Demattê et al. 2018; Žížala et al. 2019), 0.30 ((Gomez et al. 2019; Safanelli et al. 2020; Ward et al. 2020) and 0.35 (Castaldi 2021; Castaldi et al. 2019a). The choice of stricter thresholds to minimize the inclusion of pixels with disturbing effects is made at the expense of the extent of the area that can be mapped (Vaudour et al. 2021). Here, $\text{NDVI} < 0.25$

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represents a good trade-off between mappable area and effectivity (evaluated visually) to mask vegetated surfaces.

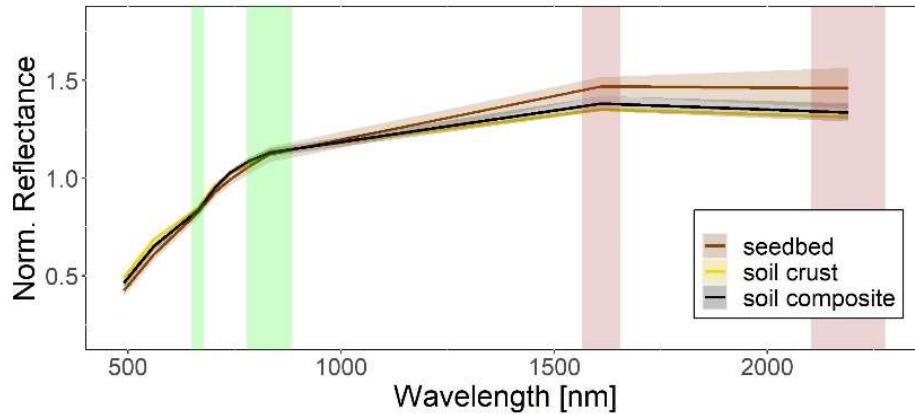


Figure 5.7: Mean S-2 spectra of the two soil surface conditions encountered in the Belgian loam-belt which are suitable for soil mapping from remote sensing: seedbed and soil crust. The black spectrum is a mean S-2 exposed soil composite spectrum of spring months 2016-2021 which is used for soil organic carbon mapping. The green vertical bands indicate the location of S-2 B4 and B8 used to calculate NDVI and the brown vertical bands are S-2 B11 and B12 used to calculate NBR2.

The NBR2 threshold to discriminate moist soils and crop residues was defined based on field observations, and was set to 0.05. Vaudour et al. (2021) used $\text{NBR2} < 0.053$ to detect bare soils. They defined the index value as the first quantile of the NBR2 distribution across S-2 images of the Versailles Plain, France. Demattê et al. (2018) stated that the use of 0.075 as NBR2 threshold provides the best association between laboratory and Landsat 5 spectra in a 14,614 km² area in southeastern Brazil. Castaldi et al. (2019a) tested different NBR2 thresholds and found that $\text{NBR2} < 0.05$ improves SOC prediction, but reduces the area for which SOC can be mapped in Demmin, Northern Germany. Ultimately, the choice of thresholds used to mask unwanted pixels is bound to have an effect on the exposed

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soil composite, whether on its quality or its spatial extent. Given that both study areas (southern Belgium and the Dutch polders) have similar climate conditions and are both dominated by intensive arable cropping systems, we assumed similar thresholds for NDVI and NBR2. In total 83% of the total cropland area was included in the exposed soil composite when using $NDVI < 0.25$ and $NBR2 < 0.05$. The number of observations per pixel varied, with 18% of pixels having less than seven observations per pixel (Figure 5.8).

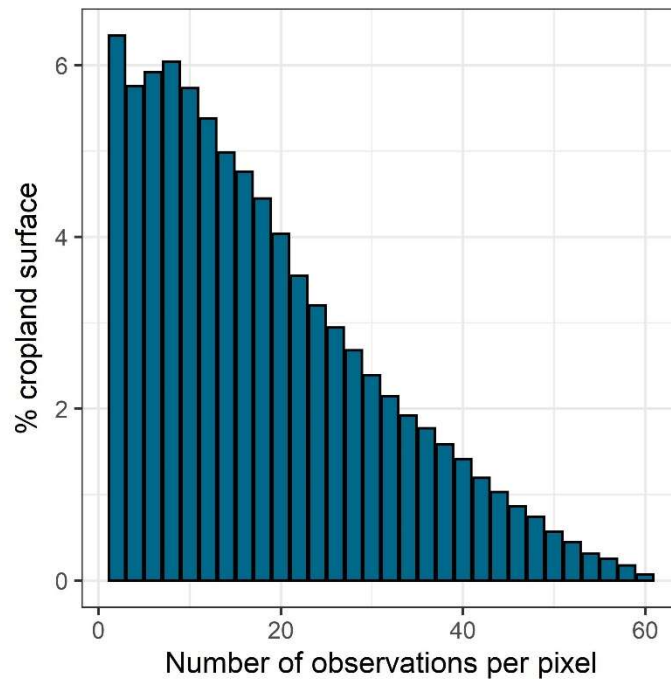


Figure 5.8: *Percentage of mapped cropland surface by the exposed soil composite in southern Belgium and the Netherlands for groups of pixels with the same number of observations.*

5.3.3 SOC prediction models

The general statistics of the calibration datasets and the two independent validation datasets are shown in Table 5.2 and Figure 5.9. The SOC content of the 124 calibration points was on average 14.2 g C kg^{-1} and was rather variable: variation coefficient (CV) of 29% (Table 5.2). The exposed soil composite obtained in section 4.2.4 provided a good basis for SOC mapping over large areas. The average prediction accuracy of the 100 ten-fold-cross validation runs yielded an MEC of 0.48 ± 0.07 , RMSE of $3.4 \pm 0.6 \text{ g C kg}^{-1}$, RPD of 1.4 ± 0.2 and RPIQ of 2.0 ± 0.3 (Figure 5.10A). In 71% of all cases, the best performance of the PLSR model was obtained when using four LVs. The accuracy is comparable to the one obtained by Vaudour et al. (2021), who applied an NBR2 threshold to S-2 composite imagery to create bare soil composite. They obtained $R^2 = 0.53$, $\text{RMSE} = 3.2 \text{ g C kg}^{-1}$ and $\text{RPD} = 1.46$ and covered 34.28 km^2 of croplands in the Versailles Plain, France.

The VIP pointed to the relative importance of S-2 bands B2, B11 and B12 in the model (i.e. $\text{VIP} > 1$; Figure 5.10B). This is in agreement with previous studies (Castaldi et al. 2016) and findings from Chapters 3 and 4. In particular B11 and 12 are also the ones that react to disturbing effects from residues and soil moisture. This underlines the importance of the NBR2 threshold to remove pixels with residue cover or moist pixels in order to avoid using these for SOC prediction models.

The disadvantage of the PLSR model used is its linearity, which is not suitable for the nonlinear relationship between SOC and the spectra. Therefore, we have tried two other models for SOC prediction (results not shown) : Cubist algorithm, and Convolutional Neural Network (CNN). However, the number of samples was too low for a correctly performing CNN, and Cubist algorithm did not provide a better model performance than PLSR.

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Table 5.2: General statistics of the SOC content of the model calibration (Cal) soil samples and the REQUASUD independent validation (Val) soil samples. Skewness is calculated via Fisher's moment coefficient. (SD = standard deviation, CV = coefficient of variation, Sk = Skewness)

	n	Min*	Max*	Mean*	SD*	CV (%)	Sk
Cal	124	7.2	28.2	14.2	4.9	34	1.0
Val	34,385	3.0	67.0	13.5	4.8	35	3.0

* Expressed in g C kg⁻¹

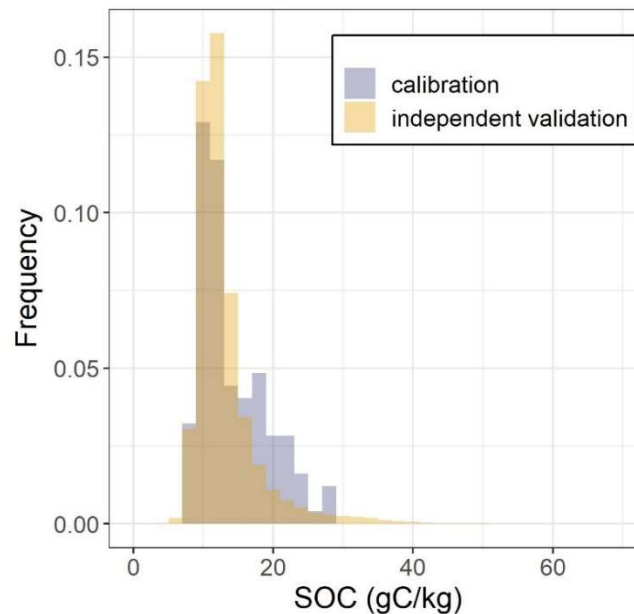
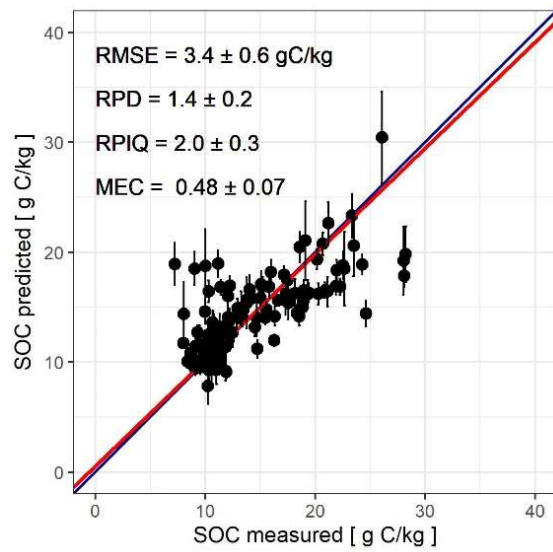
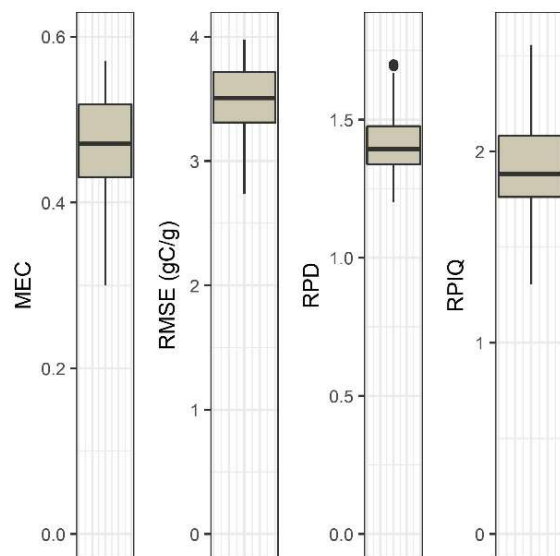


Figure 5.9: Frequency distribution of SOC contents of the model calibration dataset ($n=124$) and the external validation dataset REQUASUD ($n=34\ 385$).

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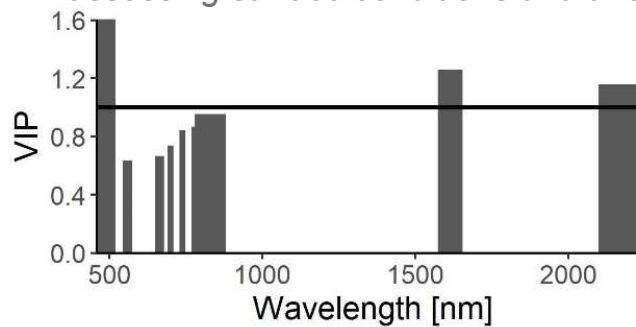


(A)



(B)

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(C)

Figure 5.10: (A) Measured against predicted SOC of one (randomly chosen) of the 100 PLSR model runs (10-fold cross validation). The model performance indicators refer to the average values of the 100 PLSR models. The blue line is the 1:1 line, the red line is the regression line. (B) Distribution of model performance indicators obtained from the 100 PLSR models. (C) Mean Variance Importance in Projection (VIP) scores for the 100 PLSR model runs. Predictors with VIP values greater than one (area above the horizontal line in the plot) were considered significant for the PLSR model. The width of the bars represents the width of the Sentinel-2 bands.

5.3.4 SOC maps and their uncertainty

Three maps were constructed: i) mean SOC content map, ii) a map of the number of scenes per pixel of the exposed soil composite and iii) a map visualizing the PIR of the SOC prediction (Figure 5.11). According to Gomez et al. (2015) there are five sources of uncertainty in soil property mapping from remote sensing: i) uncertainty of the spectra linked to device repeatability and ii) spatial positioning; iii) uncertainty of the reference lab values; and iv) uncertainty of the model building linked to the choice of calibration set and v) choice of model dimension. Here we used the bootstrapping method (100 bootstraps, section 5.2.4.2) to assess the uncertainty linked to the model building (iv). Given the spectral stability of the exposed soil composite and the radiometric stability and spatial resolution (20 m) of

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S-2 MSI (Drusch et al. 2012), the uncertainty related to the spectra (i) and its positioning (ii) was neglected. We also neglected the uncertainty related to the reference lab values (iii), as it is not strictly related to spectral modelling.

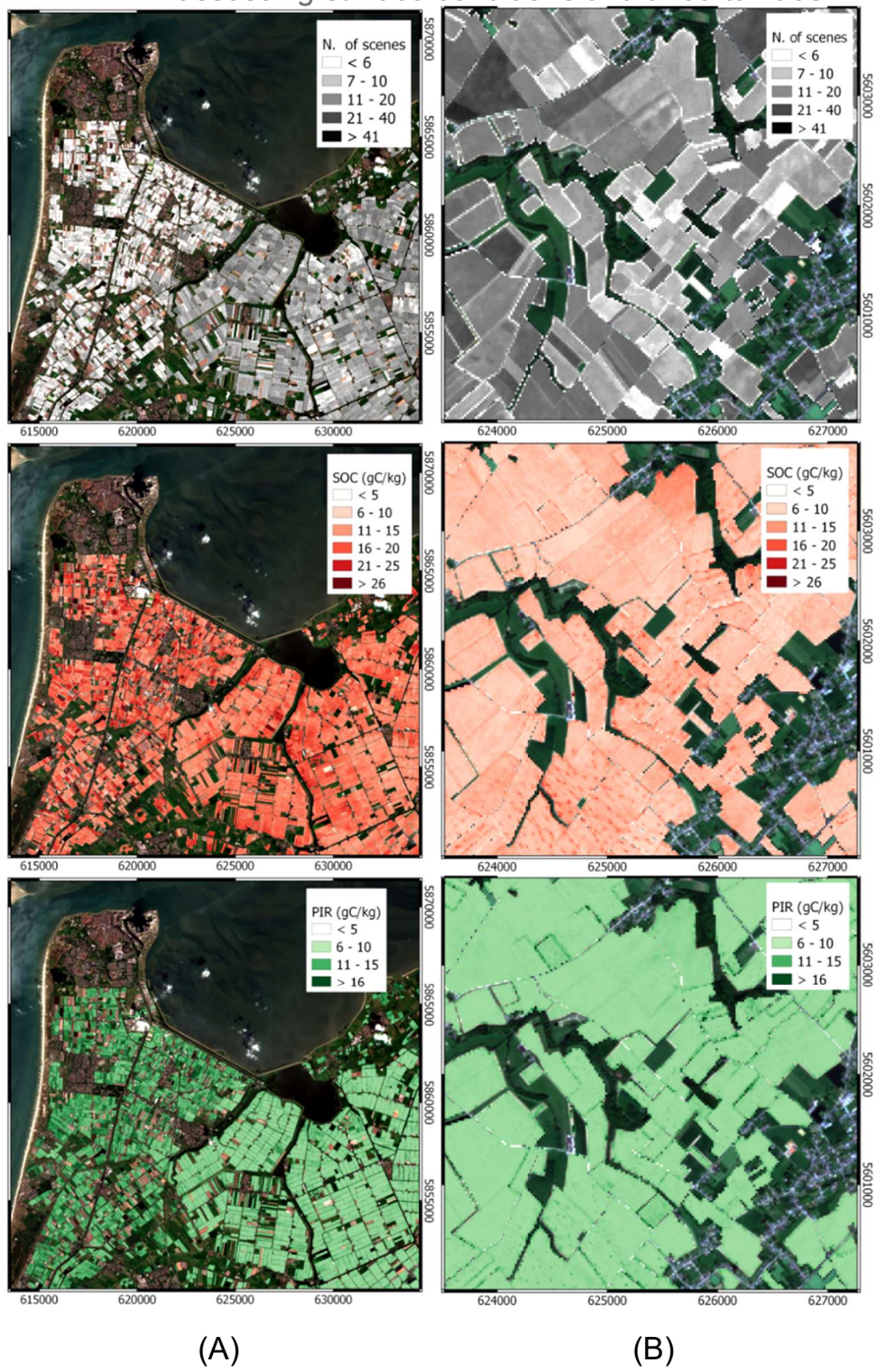
Higher uncertainty values were generally observed for field borders (Figure 5.11B bottom), where the number of contributing scenes is low (Figure 5.11B top) and pixels can represent a mixture of the surface conditions in both of the adjacent fields. Additionally, mixed pixels were excluded from the calibration dataset and the PLSR model is therefore not trained to predict mixed pixels. Several techniques exist for spectral unmixing, i.e. the separation of a pixel spectrum into its pure component endmember spectra, and the estimation of the abundance value for each endmember (Plaza et al. 2009). These techniques are however computationally intensive and require a large dataset of training samples.

The southern part of the SOC prediction map of the Belgian loam belt shows spots with higher SOC content within the fields (Figure 5.11B). These are the remains of pre-industrial charcoal kilns. On bare cropland soil, the enrichment with charcoal appears as circular black spots up to 40 m in diameter. The charcoal has been mixed through the topsoil by repeated tillage over time (Hardy et al. 2019). The uncertainty map of SOC prediction displays patterns linked to the number of scenes per pixel. Large uncertainty (average PIR = 14 g C kg⁻¹) is observed in the western part of Noord-Holland (Figure 5.11A bottom), compared to the neighboring Wieringermeer polder with smaller uncertainty (average PIR = 11 g C kg⁻¹). This large uncertainty coincides with a small number of scenes contributing to the composite map (Figure 5.11A top). This small number of scenes is linked to the early season cropping leading to high NDVI values on the spring composite. Spring-blooming bulbs, such as tulips, are widespread in the sandy region bordering the coast. Overall, it can be seen that uncertainty hardly

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decreases for pixels representing the mean spectrum of six or images (Figure 5.12). Such a threshold is not commonly specified. Castaldi (2021) for example arbitrarily chose three scenes as a minimum for an exposed soil composite and Zepp et al. (2021) suggested considering the number of cloudless scenes per pixel as an internal quality measure. We observed that setting the threshold of minimum six scenes can lower the mean PIR of the prediction maps from 15.0 to 12.4 g C kg⁻¹ (Figure 5.12). This has, however, an effect on the total surface of croplands covered by the SOC prediction map: 83% without threshold versus 65% if at least six scenes per pixel are required. The pixels for which less than six scenes are available are generally field borders (mixed pixels, Figure 5.11B), soils with bad drainage (removed by the NBR2 threshold), and fields where farming practices do not allow full exposure during spring months (removed by the NDVI or NBR2 thresholds, Figure 5.11A). This definition of minimal number of scenes will however likely vary regionally, and it is strongly depending on the type of model used and the thresholds applied. For example, different soil types encountered will react differently to NBR2, and different predictive model will affect the estimated variance of bootstrap predictions that enters in the uncertainty calculation (Equation 5.6). The selected six scenes might be too optimistic, as Heiden et al. (2022) recommend a minimum of 7–15 observations per pixel, depending on the spectral index used for the composite creation.

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Figure 5.11: Comparison of the spatial patterns (from top to bottom) of the number of scenes per pixel, the predicted SOC and the uncertainty (expressed by PIR; see Equations 5.6-5.10) of the SOC predictions resulting from partial least squares regression model with 100-fold bootstrapping. (A) Noord-Holland in the Netherlands, (B) fields in the vicinity of Beuzet village in the Walloon region Belgium). Grid units are in meters from the origin of the projection. Projection: Transverse Mercator, Projected coordinate system: WGS_1984_UTM_Zone31N.

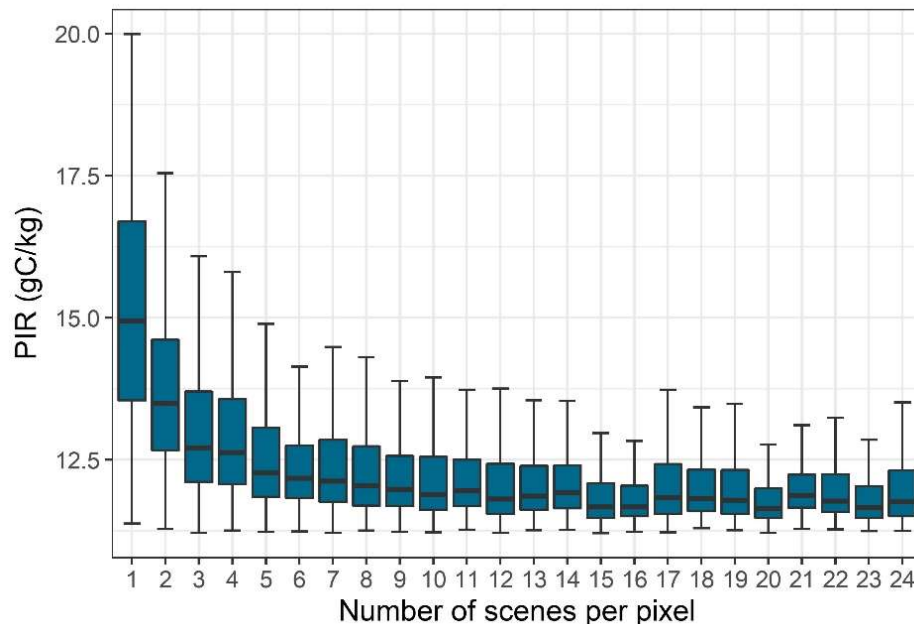
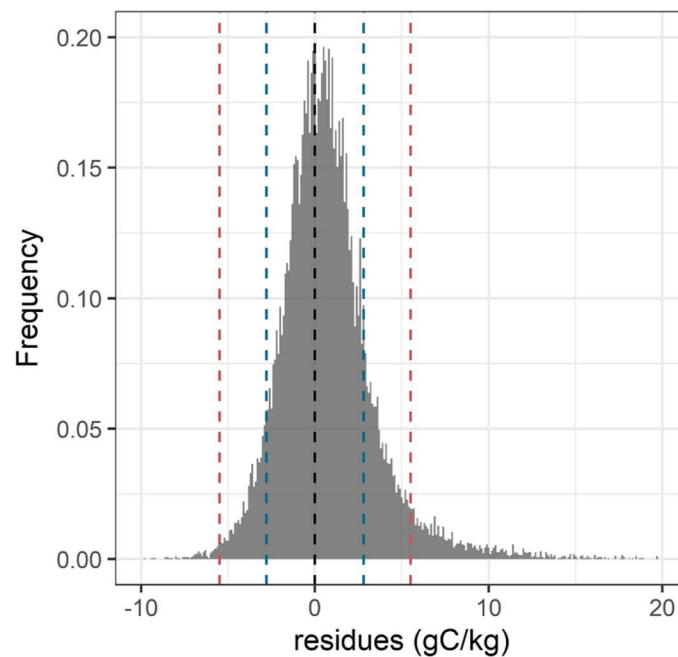


Figure 5.12: The uncertainty (expressed by Prediction Interval Ratio (PIR); Equations 5.6-5.10) of 100 soil organic carbon (SOC) predictions resulting from a partial least squares regression model with 50-fold bootstrapping as function of the number of scenes per pixel in the exposed soil composite used for SOC prediction.

A map of the mean SOC content per field was constructed by averaging SOC predicted values per field entity, to allow the validation with REQUASUD external validation dataset.

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The coverage of the mean SOC map is lower than the one of the per pixel map. This is because for a number of fields the conditions for predicting the SOC were not met i.e. number of scenes per pixel > 5, minimal count of pixels per field unit, or both. Therefore, the mean SOC value per field (Table 5.3) differs slightly from mean SOC per pixel. The validation against an independent dataset with 34,385 samples (REQUASUD) showed a Gaussian distribution with a relatively small bias of $0.5 \text{ g C kg}^{-1} \pm 2.8 \text{ g C kg}^{-1}$ (Figure 5.12). From the distribution it can be seen that 95% ($1.96 \times \text{SD}$) of fields are correctly predicted within an interval of $\pm 5.5 \text{ g C kg}^{-1}$ and 68% ($1 \times \text{SD}$) of samples are correctly predicted within the interval of $\pm 2.8 \text{ g C kg}^{-1}$.



Source: Base de données REQUASUD

Licence n.: A07/2021

Figure 5.13: A comparison of the residues between the predicted and the measured SOC contents of the external validation dataset obtained from REQUASUD. The blue dashed line is $1 \times \text{SD}$, the red dashed line $1.96 \times \text{SD}$.

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Table 5.3: Statistics of the SOC content prediction and the Prediction interval ratio (PIR) for the pixel-based approach and for field-based approach. (SD = standard deviation)

Approach	n		mean	median	SD
Per-pixel	11 235 492 pixels	SOC*	14.1	13.3	4.7
		PIR*	12.4	11.8	1.6
Per-field	92 451 fields	SOC*	13.6	12.7	3.2
		Residues*	0.7	0.5	2.8

* Expressed in g C kg⁻¹

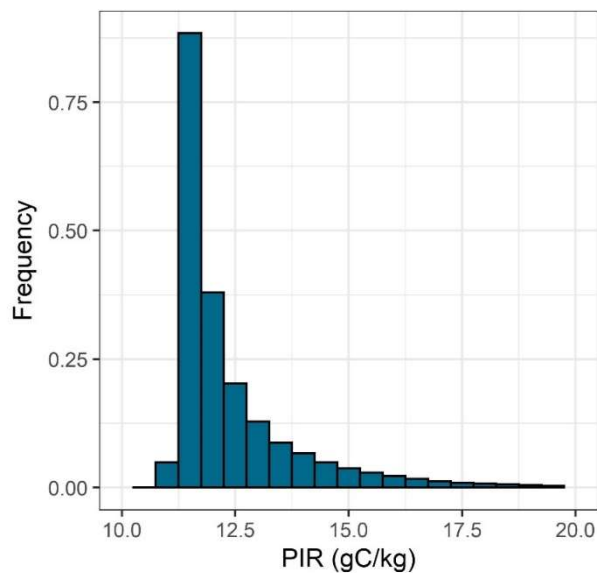


Figure 5.14: Distributions of the uncertainty (expressed by Prediction Interval Ratio (PIR), Equations 5.6-5.10) of 100 soil

Improving SOC predictions from a Sentinel-2 composite by assessing surface conditions and uncertainties organic carbon (SOC) predictions resulting from a partial least squares regression model with 100-fold bootstrapping performed at the scale of a pixel in southern Belgium loam belt and the Dutch polders (for the extent of croplands see Figure 5.1).

For the mean SOC content per field, 95% of samples have an error below 5.5 g C kg^{-1} (Table 5.3). The good performance of the SOC prediction for a large area (5 370 km² of croplands) is partially attributed to the similarity of soil types, and the low SOC contents (the measured SOC values range from 5 to 30 g C kg^{-1}), making a single PLSR model sufficient to capture the variability. For a larger area, splitting into several models based on ancillary variables (e.g. soil type or principal component analysis) (Castaldi et al. 2019c; Stevens et al. 2012) or using a local calibration approach, such as Ward et al. (2020) did, should be considered.

Overall, a five-year S-2 spring composite image has shown to be appropriate for SOC prediction of loamy soils in Belgium and the Dutch polders with 5.5 g C kg^{-1} accuracy at the field level. SOC monitoring, however, relies on repeatability over time, with as main purpose change detection (Andries et al. 2021). This requires consistency of calibration and validation datasets, and suitable accuracy. As a matter of fact, comparison between 2009 and 2015 LUCAS surveys showed limited changes in SOC over the six years period (Fernandez Ugalde et al. 2020). The pixel SOC prediction map demonstrated large uncertainty: mean PIR = 12.4 g C kg^{-1} , while mean predicted SOC = 14.1 g C kg^{-1} (Table 5.3, Figure 5.13). Hence, PIR represents on average 88% of the predicted SOC value. While the mean SOC map might be a useful product to quantify average SOC at regional or national level, local soil monitoring of SOC is rendered obsolete with such high PIR values (Kempen et al. 2019). As suggested by Chen et al. (2022), it should be discussed whether PIR should be calculated at

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90% prediction intervals, or should be narrower to be useful for decision-making. For some decision makers, 75% prediction interval might be adequate to support a decision (Chen et al. 2022). Validating models by region is an alternative to improving the uncertainty, as regional MSE tend to be lower (Brungard et al. 2021). Lower MSE decreases the variance (Equation 5.6), resulting in an overall lower uncertainty.

The accuracy of SOC content prediction maps at field level ($\pm 2.8 \text{ g C kg}^{-1}$; Table 5.3) should in theory be small enough to detect the effects of management practices on SOC contents in the short to mid-term (5-10 years). In fact, van Wesemael et al. (2019) have shown that fields in the Belgian Loam belt converted to conservation agriculture for at least 10 years had more than 4 g C kg^{-1} higher SOC contents than comparable fields under conventional agriculture. The average SOC contents per field can be used for decision making at the regional scale e.g. to characterize the SOC contents in croplands for a region with similar soils and climate or as a proxy for SOC stocks. Obviously, the bulk density, vertical gradient in SOC content and the stone content are additional variables that are not provided by the current spectroscopic approach. Garten Jr and Wulfschleger (1999) were among the first to calculate a minimum detectable difference (MDD) for SOC inventories. MDD determines the level of SOC change that could theoretically be detected for each unit. The challenge associated with MDD is the large number of independent soils samples that is required (Smith et al. 2020). The UN Sustainable Development Goal (SDG) 15.3.1 defines areas of degraded land as the ones suffering from more than 10% average net reduction in SOC stocks (Sims et al. 2020). Here we provide a large inventory of SOC content data that could be used as a proxy for SOC stock in such MDD calculations. For example, the MDD of the SOC content prediction of 1000 randomly sampled fields (selected by conditioned Latin hypercube on spatial coordinates,

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Minasny and McBratney (2006)) in the Loam belt is 0.35 g C kg^{-1} for an average SOC content of 12.5 g C kg^{-1} . This means that SOC content change of 2.8% can be detected, which is well below the 10% of the SDG 15.3.1.

It remains to be seen whether the detection limit of SOC prediction models from exposed soil composite is low enough to detect SOC stock changes in croplands, and what the appropriate period of time is to acquire a minimum of six valid scenes per pixels in the exposed soil composite. Furthermore, the methodology used for SOC modelling has to be consistent in every way, if a time series of SOC maps is to be compiled. As addressed by Zepp et al. (2021), larger and standardized validation and calibration datasets are needed, to produce large-scale SOC predictions (national to European-wide), in a consistent manner. It is also important to note that the time range between satellite imagery collection and the sampling period should be reduced to minimum, to exclude low quality training data at the calibration step. A compromise needs to be found between the length of the compositing period and the dates of the sampling. Last but not least, de Gruijter et al. (2016) have shown that SOC prediction maps and associated error variances can be used as a source of univariate information for stratification sampling. Taking prediction errors into account in soil sampling strategy minimizes sampling variance and creates optimized stratification, leading to better performing models (de Gruijter et al. 2016).

5.4 CONCLUSION

Earth observation serves as a valuable base for digital soil mapping, as satellite images allow monitoring over time and over large areas with a resolution that allows distinguishing within and between field patterns. Creating an exposed soil composite, i.e. stacking several spatially overlapping images into one composite image based on an aggregation function, allows combining all exposed soils of all input

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scenes, thus increasing their extent. The resulting composite spectrum however does not necessarily reflect the pure soil signal at least for an important fraction of the cropland area. We have found that applying an $\text{NBR2} < 0.05$ threshold and normalizing the S-2 spectra allow obtaining a reasonable soil reflectance signal, where crop residues and moist soils are excluded, and crusts are corrected for. Using these criteria in Google Earth engine, we built an exposed soil composite from Sentinel-2 imagery (covering the spring periods of 2016-2021), mapping 5 370 km² of croplands in Belgium and the Netherlands. The exposed soil composite was used to produce SOC prediction maps, accompanied by a measure of uncertainty. This compositing method showed both realistic within field and regional SOC patterns. An accuracy of 5.5 g C kg⁻¹ was reached at the field level for 95% of samples. The uncertainty of prediction was assessed via the PIR. On average, PIR represented 88% of the predicted SOC value. Such high uncertainty values render local SOC monitoring obsolete, however given the high accuracy of the SOC map, it may be a useful product to quantify average SOC at regional and national level.

CHAPTER 6. EVALUATING THE EFFECTS OF CONSERVATION AGRICULTURE AND CARBON FARMING ON SOC CONTENT IN CROPLANDS⁴

OUTLINE

As mentioned in Chapter 2, there is a strong motivation for the inclusion of soil-centric mitigation projects that turn agricultural soils into carbon (C) sink, to reach the Paris Agreement goal of 2030. Soil C sequestration strategies rely on management practices that increase the amount of carbon stored as soil organic carbon. Two examples of soil C sequestration strategies is conservation agriculture (CA) and carbon farming (CF). Long term experiments that quantify the effects of CA or CF on soil C sequestration however work under controlled environmental conditions, and cannot cover the huge diversity of management options available to farmers. In this chapter, we put the results from Chapter 5 in practical use. We evaluate whether soil organic carbon (SOC) maps produced in Chapter 5 can be used as a tool for a result-based incentive scheme in Walloon croplands. The advantage of such approach is the observation of realistic applications of CA and CF where environment is not controlled. Firstly, two databases are gathered which contain fields under CA and CF practices. Then, we use a matching procedure to control for covariates and obtain estimates of the impact of each practice on SOC content. We show that in 90.1% of cases the accuracy of mean SOC map produced from Sentinel-2 composite imagery (5.5 g C kg^{-1}) is too low to detect changes in SOC

⁴ The content of this chapter will be submitted as Dvorakova, K., Ferdinand, M.S. van Wesemael, J., Baret, P.V., Chabrillat, S., van Wesemael, B. Evaluating the effects of conservation agriculture and carbon farming on SOC content in croplands, using Sentinel-2 composite imagery

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which are due to CA or CF farming practices. To bypass the low accuracy, we exploit the potential of bootstrapping. Using a distribution of 100 SOC predictions, we test (Student's t-test) the significant difference between the treated and control groups. Results show that 74.2% of plots from the CA and CF databases show a statistically significant difference to their control group. Therefore, by using the large quantity of data available from remote sensing, we are able to bypass the issue of low accuracy of remote sensing data. However, limitations still exist, notably the lack of a full spatial coverage, and the use of SOC content as indicator, and not SOC stock as required in GHG budgets.

6.1 INTRODUCTION

Agri-food systems account for 31 percent of global greenhouse gas (GHG) emissions, composed of 13 percent from activities within the farm gate, 7 percent from land use change processes and 11 percent from pre- and post-production processes (FAO 2021). The Intergovernmental Panel on Climate Change (IPCC) stated that land degradation in agricultural systems can be addressed through sustainable land management with an ecological and socioeconomic focus, with co-benefits for climate change adaptation (Shukla et al. 2019). Together with the Food and Agriculture Organization (FAO), they promote the adoption of Conservation Agriculture (CA) as a sustainable management practice that achieves a balance of agricultural, economic and environmental benefits (Dumanski et al. 2006). On the one hand, CA increases the resilience of agricultural productivity through increasing organic matter (consisting for 58% of carbon), which improves the water and nutrient retention capacity and strengthens the soil structure (Sharma et al. 2021). On the other hand, the aforementioned increase in organic matter results from an increase in biomass production and/or a

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decrease in mineralization. Both processes induce a decrease of atmospheric CO₂ by increased photosynthesis (biomass production) or decreased heterotrophic respiration (mineralization) (Sharma et al. 2021).

CA is based on three pillars: (1) minimal soil disturbance (i.e. no-tillage or reduced tillage), (2) continuous soil cover with the use of cover crops and/or crop residues and (3) diversification of plant species through varied crop rotations, crop associations, intercrops or varietal mixtures (FAO 2022). CA implies the application of the three pillars at the same time. However, as suggested by Valkama et al. (2020), classical long-term experiments investigate the effect of each of these pillars separately and studies on the beneficial effects of combining different measures are rare. This leads to questioning the efficacy of CA to store carbon (C) in agricultural soils (Giller et al. 2015; Valkama et al. 2020). While no- or reduced- tillage implementation (pillar 1) by itself has positive influence on soil organic carbon (SOC) stock in the upper soil layer (0-15 cm), the effects on SOC stocks in the upper 30cm and deeper are non-significant (Chenu et al. 2019). Hence, no increase in SOC stock for the land unit is detected if the whole profile is considered. Contrarily, the combination of no- or reduced- till with the two additional pillars has shown to have beneficial effect on SOC stocks throughout the entire profile (Chenu et al. 2019). Continuous soil cover (pillar 2) provides additional organic carbon (OC) inputs to the soil, which is the best option to increase SOC stocks (Chenu et al. 2019; Valkama et al. 2020). Additionally, diversification of plant species (pillar 3) causes a diversification of the quality of the C inputs, which is, especially in case of legumes, particularly efficient in increasing SOC stocks (Chenu et al. 2019). Nevertheless, meta-analysis and literature reviews of long-term experiments reveal inconsistent effects of CA (Giller et al. 2015). Additionally, while being indispensable, long term experiments cannot cover the huge diversity of

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management options available to farmers (Chenu et al. 2019).

Recently, as part of the Green Deal 2019, the European Union (EU) has proposed a legislative framework for sustainable food systems, the Farm to Fork Strategy. The strategy aims to accelerate the transition to a sustainable food systems to mitigate climate change and ensure food security (COWI 2021). One of the pivot points of The Farm to Fork Strategy is Carbon Farming (CF). In CF, farmers are offered incentives to improve their farming practices and safeguard the environment, through the application of mitigation actions at farm level to manage carbon and GHG fluxes. A few examples of mitigation actions identified to be relevant for carbon farming for cropland management are (i) reduced tillage, (ii) use of cover crops, (iii) leaving crop residues on the soil surface, (iv) improved crop rotations and (v) ceasing to burn crop residues and vegetation (COWI 2021). The main difference between CF and CA is that while the examples of CF mitigation actions overlap with the three pillars of CA, their application is free of choice and no rule exists which states that they have to be applied at the same time, contrarily to CA.

There are various ways to reward famers for improving their farming practices. The most commonly offered incentives are action-based payments (COWI 2021). Farmers are paid for actions they either take or refrain from, for which there is evidence of a link to sequestration, preserving SOC stocks in the case of peatlands or organic soils or reduction in GHG emission (COWI 2021). Adversely, very few schemes offer result-based payments (COWI 2021). The incentive is linked to the measured outcome of the farming practices that are applied (COWI 2021). The disadvantage of the result-based scheme is the exposure of the famer to the risk of non-delivery, resulting in a higher financial risk and uncertainty for the farmer (COWI 2021).

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In mineral agricultural soils, maintaining, or better, enhancing the existing SOC levels is crucial, given that SOC is closely related to soil health, water holding capacity and stability of yields, and the estimated EU emissions from mineral soils under cropland are important at 27 Tg CO₂eq (COWI 2021). This makes SOC a suitable indicator for CF result-based schemes. In Chapter 5 we have used freely available Sentinel-2 satellite imagery to map SOC content in croplands over areas larger than 5000 km². The produced maps correctly showed regional variations in SOC content in croplands.

Here we evaluate (i) whether CA and action-based CF have beneficial effects on SOC content in Belgian croplands, and (ii) whether the accuracy of SOC map produced from Sentinel-2 composite imagery is good enough to distinguish between CA and CF fields on the one hand and comparable fields under conventional agriculture on the other hand. The advantage of using remote sensing is the inclusion of field observations that reflect reality, contrarily to the long-term trials effectuated under controlled management practices with treatments unchanged for several years (Chenu et al. 2019; Valkama et al. 2020). We have used two datasets: one containing 307 fields which fall under CA, and one dataset of 435 fields which are part of an action-based CF. Given that the SOC sequestration potential varies considerably at farm level because of the heterogeneity of soils and climatic conditions, we made use of statistical matching technique to control for covariates, where variation in SOC content is compared between treatment and control group. The response ratio (RR), which represents the percentage change, is calculated for each matched pair.

6.2 MATERIALS AND METHODS

The study was conducted in Wallonia, southern Belgium, covering an area of 16 900 km², described in section 2.5.2.

6.2.1 Conservation Agriculture survey

Since there is no list of CA farms in Wallonia, we carried out a survey on the adoption of CA in collaboration with twelve public and private institutions, eight farmers' associations, two researchers from Belgian universities but also by snowball method with the CA farmers already met by the Sytra laboratory and through the use of the social network Facebook (Ferdinand and Baret, 2024). Snowball method is a purposive sampling method for selecting new participants according to the description of the participants already interviewed (Tiftonell et al. 2020; Tessier et al. 2021). Based on the survey results 221 Walloon farmers were contacted. A verification of CA practice through telephone interviews and cross-referencing was then carried out. Since reducing tillage is the main gateway for farmers to start a transition (Vankeerberghen and Stassart 2014), only farmers practicing direct seeding (no soil disturbance), no-till (no inversion) or reduced till (inversion but not every year and/or to a depth of less than 20cm), were considered to practice CA. This audit reduced the number of farmers practicing CA in 2020 resulting from the survey to 190 farmers. The majority (85%) were located in the Sandy-loam, Loam and Condroz regions (Figure 6.1).

To further reduce the work load, farmers were selected based on four criteria. The first criterion requires a minimum five years practice of CA. According to Hobbs (2007), it takes between three and seven years of practice for the benefits of CA to appear. Additionally, the study by Derrouch et al. (2020) showed that farmers needed about five years to adapt and start mastering the CA system. Hence, this first filter helped to rule out recent adopters of CA, whose farming practices were still evolving and the effects of which may not yet be reflected in the SOC contents. Then, in order to maximize the diversity of CA practices, purposive sampling (i.e. a form of nonprobability sampling in which the researcher deliberately selects

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individuals from the population whom he expects to give the most information (Wauters and Mathijs 2013)) was performed on farmers with more than five years of CA experience. The criteria were three-fold: (i) geographical distribution, (ii) organic certification and (iii) livestock ownership.

(i) Given the intensive agricultural practices in the Sandy-loam, Loam and Condroz agricultural regions (containing 80% of all croplands in Wallonia), these regions are at a high risk of water erosion in croplands with low organic matter content (Biielders et al. 2003). Consequently, farmers in the Sandy-loam, Loam and Condroz agricultural regions were the first to adopt CA and it is now widespread in these regions. In southern Wallonia, practicing CA is attractive to protect the soils from severe water erosion related to the rugged terrain and high erosivity of rainfall (Maugnard et al. 2013), as well as the difficulty of working some (stony) soils (Dannevoye et al. 2013). Overall, farmers' motivations and soil conservation practices may differ, as each agricultural region has specific characteristics that influence the agro-economic potential of its farmland and thus the type of agriculture that develops there (Goidts and van Wesemael 2007). This is why we tried to cover as many different agricultural regions as possible in the survey. Note, however, that it was not possible to find a CA farmer with more than five years of experience in each region.

(ii) In order to be inclusive, farmers practicing CA under organic certification were included. While crop diversification is a central concept in organic agriculture, reduced tillage is more complicated due to the importance of tillage for weed control (Cooper et al. 2016). Therefore, different strategies must be employed, involving changes in CA practices.

(iii) According to FAO (2022), CA offers a greater possibility of crop-livestock association. This association can lead to an increase in the share of catch crops (cover crops to be

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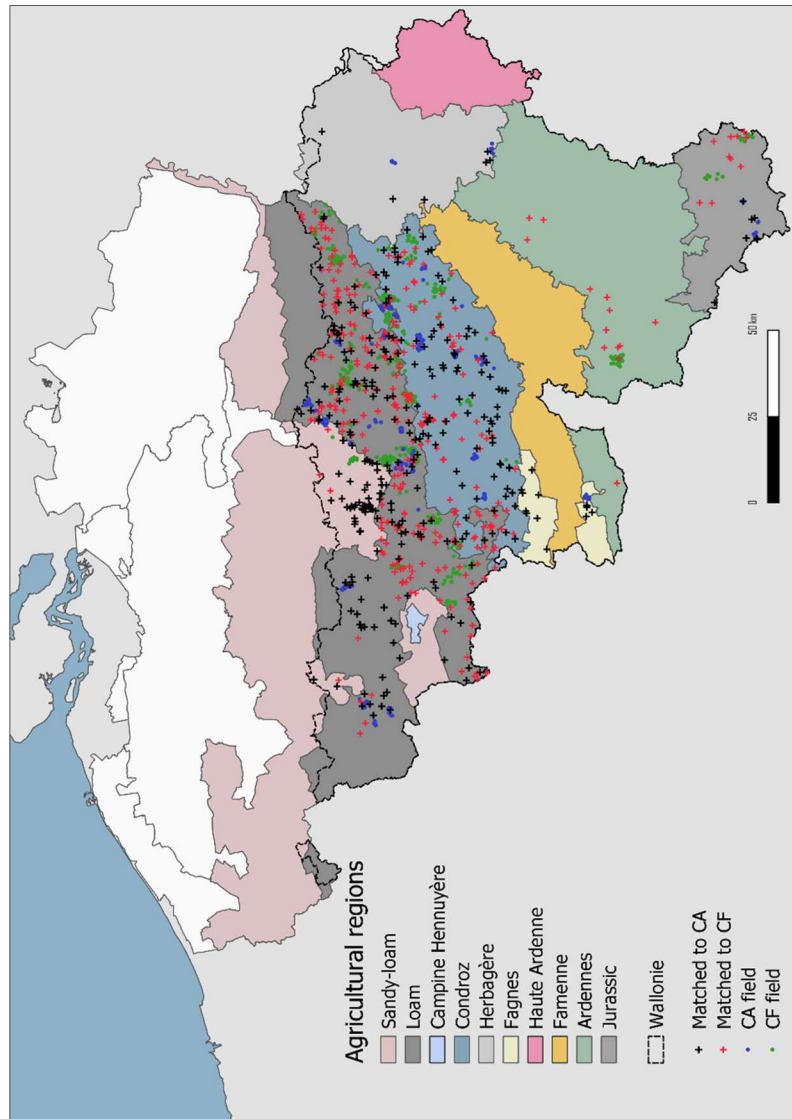


Figure 6.1: *Delineation of the official agricultural regions in Belgium, overlapped by the administrative limits of the Walloon region, and the locations of the studied fields. CA = conservation agriculture, CF = carbon farming.*

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We interviewed 28 farmers, distributed over six agricultural regions (Table 6.1). Eighteen of them (64%) have livestock and nine (32%) have certified organic fields. During semi-structured interviews, conducted between November 2021 and February 2022, 307 fields under CA belonging to these farmers were identified. 89% of the fields were located in the Sandy-loam, Loam and Condroz regions (Ferdinand and Baret, 2024; Figure 6.1). During the survey, three additional variables were reported for each farmer: (i) the possession of livestock (binary), (ii) type of tillage (no-till, reduced till) and (iii) the year of conversion from conventional agriculture to CA.

Table 6.1: *Geographical distribution of the Walloon Conservation Agriculture (CA) population according to the different agricultural regions (see Figure 6.1 for their location). O = organic, NO = non-organic.*

Agricultural region	Population	Final sample			
	n CA farmers	n CA farmers		n fields	
		O	NO	O	NO
Sandy Loam	13	0	3	0	61
Loam	103	5	7	42	59
Campine Hennuyère	0	0	0	0	0
Condroz	45	2	6	36	75
Herbagère	3	0	2	0	11
Fagnes	4	1	0	15	0
Famenne	3	0	0	0	0
Haute Ardenne	3	0	0	0	0
Ardenne	4	0	0	0	0
Jurassic	5	1	1	4	4
Total	183	9	19	97	210

6.2.2 Carbon Farming database

The dataset of farmers practicing CF was obtained from an independent agricultural advisor Soil Capital©. Soil Capital

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launched a certified multinational carbon payment program for French and Belgian farmers in 2020, to help them with the transition to more profitable and regenerative agriculture by giving the chance to earn carbon certificates. The program targets arable farmers with more than 100 ha, with no requirement for a priori CF activity. Soil Capital uses the Cool Farm Tool to measure the GHG balance across the entire farm (Hillier et al. 2011). The Cool Farm Tool requires inputs of which farmers typically have good knowledge: (i) crop management (geographic location, crop yields, soil properties, tillage practice, C input class, fertilizer and crop protection usage), (ii) livestock and manure management, (iii) field energy use and (iv) primary processing energy use (Hillier et al. 2011). It combines several established empirical models for GHG emissions to give a single overall estimate based on current and previous farming practice (Hillier et al. 2011). For farmers who are net emitters according to the Cool Farm Tool, Soil Capital generates annual certificates for reductions in emissions and improved sequestration after adoption of CF practices compared to the benchmark of their initial practices. For farmers that are already sequestering, Soil Capital compares the farm against a standard baseline figure for similar farms in the region, and generates certificates based on the difference. This part of the process is fully action-based. Additionally, Soil Capital creates a positive financial incentive to retain the sequestered carbon for at least 10 years i.e. 20% of the generated certificates are retained by Soil Capital for 10 years. During the retention period, the farms are monitored, and only if there is no detected risk of carbon being released are the remaining 20% of certificates sold. In total, the CF database contains 435 fields, 89% of which are located in the Sandy-loam and Condroz regions. For each field, the CF provides four relevant variables to this study: (i) type of tillage (no-till (including direct seeding), reduced till (soil inversion to less than 20 cm depth) or conventional till (soil inversion to more than 20 cm depth)), (ii) cover crops use (binary), (iii) tillage journey (i.e. whether the farmer has

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changed the type of tillage, and if so, year of the change) and, (iv) organic fertilizer application (binary).

For the remainder of the analysis, we chose to group direct seeding and no-till. On the one hand, because the CF database does not distinguish between direct seeding and no-till. On the other hand, because, unlike no-till, direct seeding is difficult to achieve on all the crops in the rotation. For example, some CA farmers use direct seeding for crops such as cereals, rape or temporary grassland, but will need some degree of tillage for more demanding crops such as vegetables or root crops. In addition, poor weather conditions may prevent the farmer from direct seeding and require the farmer to prepare the soil before seeding.

6.2.3 SOC map

The SOC values per field were extracted from SOC map produced in Chapter 5. To summarize, the results of a validation of the SOC prediction against an independent data set showed a median difference of $0.5 \text{ g C kg}^{-1} \pm 2.8 \text{ g C kg}^{-1}$ SOC between the measured (average SOC content 13.5 g C kg^{-1}) and predicted SOC contents at field scale. This means that 68% ($1 \times \text{SD}$) of fields were correctly predicted within the interval of $\pm 2.8 \text{ g C kg}^{-1}$, and 95% ($1.96 \times \text{SD}$) of fields were correctly predicted within an interval of $\pm 5.5 \text{ g C kg}^{-1}$.

6.2.4 Matching

The SOC sequestration potential varies considerably at farm level because of the heterogeneity of soils and climatic conditions. To overcome this problem, we used a matching technique to control for the soil and climatic variables that may play role in the SOC sequestration potential. This resulted in matching pairs of a treated observation (in this case fields under CF or CA) with an untreated observation (conventional fields). The control variables were the clay

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content (%) obtained from the Public Administration of Wallonia (<http://geoportail.wallonie.be>, accessed date: 28 April 2022), and mean annual temperature (°C), elevation (m), annual precipitations (mm) and agricultural region obtained from Chartin et al. (2017). Except for the agricultural region vectorial dataset, the control variables were provided in the form of a raster with 50 m spatial resolution. The climatic variables were square root transformed to ensure a normal distribution. As the control variables are continuous (except for agricultural region), an exact match between paired observations is not feasible (Bruggeman et al. 2015). Therefore, the matching method must find the best balance between treatment and control groups for each covariate (Bruggeman et al. 2015). An exact match was requested for the agricultural region variable.

The paired untreated observations were selected from a dataset containing all agricultural fields for which the SOC prediction was available, excluding the fields contained in either the CA or CF database. This is based on the underlying hypothesis that any field in Walloon region that is not included in the CA or CF database is a conventional field with no specific SOC sequestration management. In total, 106 040 fields were available to select from. The nearest neighbor matching with replacement was performed with the MatchIt package available in the R software (2014). The distance measure between control and treated units was the Mahalanobis distance. Kolmogorov–Smirnov (KS) tests were used to verify the balance of covariates between matched pairs. Significance at the 0.05 level for KS tests was used.

The mean SOC content (g kg^{-1}) was extracted from the SOC prediction map produced in Chapter 5 for each treated and untreated observation. The relative values were then compared per agricultural region by means of the Response Ratio (RR) given by:

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$$RR = \frac{SOC_{treated} - SOC_{matched}}{SOC_{match}} \times 100 \quad (\text{Equation 6.1})$$

where $SOC_{treated}$ is the SOC content of a field under CF or CA and $SOC_{matched}$ is the SOC content of the paired untreated field. The RR represents the percentage change based on the comparison of results between a management practice (CA or CF) against a reference treatment (here the matched untreated fields). One sided Student's t-tests were used to verify whether calculated regional RR is significantly different from 0 ($\alpha = 0.05$). The Student's t-test was then also applied to verify whether CA and CF have different RRs within the same region. The normality of the populations was verified using Shapiro-Wilk test.

The absolute SOC difference between treated and matched field was calculated for each pair:

$$Absolute\ difference = Abs(SOC_{treated} - SOC_{matched})$$

(Equation 6.2)

If this absolute difference was larger than the SOC map accuracy, in other words the detection limit ($\pm 5.5 \text{ g C kg}^{-1}$ at 95% confidence), the difference between treated and matched sample was considered meaningful.

To fully exploit the potential of the 100-fold bootstrapping methodology used in Chapter 5, 100 SOC predictions resulting from a bootstrapped calibration dataset were extracted for each of the treated and matched fields. Instead of one SOC content value for each field, a distribution of 100 SOC values was available. This allowed to perform Student's t-tests that examine whether the population means of treated and matched fields differ from one another ($\alpha = 0.05$).

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It is important to know the limits of this approach when used for decision making such as in the framework of an MRV system. There are mainly two limits encountered in our methodology: (i) the risk of rewarding CA and CF farmers whose management practices have no or a negative impact on the SOC content of their fields (false positive), and (ii) the risk of not rewarding CA and CF farmers with beneficial management practices and therefore penalizing the farmers (false negative). Therefore, using Student's t-tests, we quantify the number of fields in the CA and CF databases whose SOC content was wrongly estimated by the SOC map. Hobbs (2007) and Derrouch et al. (2020) both established that a starting period of at least five years is necessary before the effects of improved management reflects in the SOC contents. Therefore, CF fields that have not converted to reduced or no- till or that have converted less than five years ago will likely not show increase in SOC content yet. Therefore, we expect that Student's t-test will not detect any SOC difference in CF fields younger than five years compared to conventional fields.

6.3 RESULT AND DISCUSSION

6.3.1 CA and CF datasets

No-till is practiced in 71% of the fields under CA (Table 6.2). A little more than half (53 %) are mixed farms with livestock. In the remaining 29%, the tillage depth is 20 cm (in 73% of the fields) and less than 15 cm (in 27% of the fields). Livestock possession is uniformly distributed (54% have livestock, against 46% with no livestock). Due to our selection criteria of CA farmers (see section 6.2.1) all fields have been under CA for more than five years. Somewhat less than half (45%) of the fields have been under CA practice for more than 25 years (Figure 6.2A).

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Table 6.2: *Number of fields for additional characteristics of farming systems contained in the conservation agriculture (CA, n=307) and carbon farming (CF, n=435) databases. NA= not applicable.*

	No-till	Reduced till	Conv. till	Total
CA (N)	220	87	NA	307
Tillage depth < 15 cm (%)	NA	27%	NA	NA
Mixed farming (%)	33%	63%	NA	54%
CF (N)	32	237	166	435
Cover crops (%)	28%	82%	99%	85%
Organic fertilizer (%)	0%	30%	43%	33%

Conventional mouldboard ploughing is still practiced in 38% of the CF fields, while no till is only practiced on 7% of the fields (Table 6.2). Farmers from 164 fields out of 435 (38%) have changed their tillage system and have converted from conventional to reduced till or no-till. For 50% of the fields (83 fields out of 164) this conversion took place less than five years ago (Figure 6.2B). 85% of farmers apply cover crops, and 33% apply organic fertilizer.

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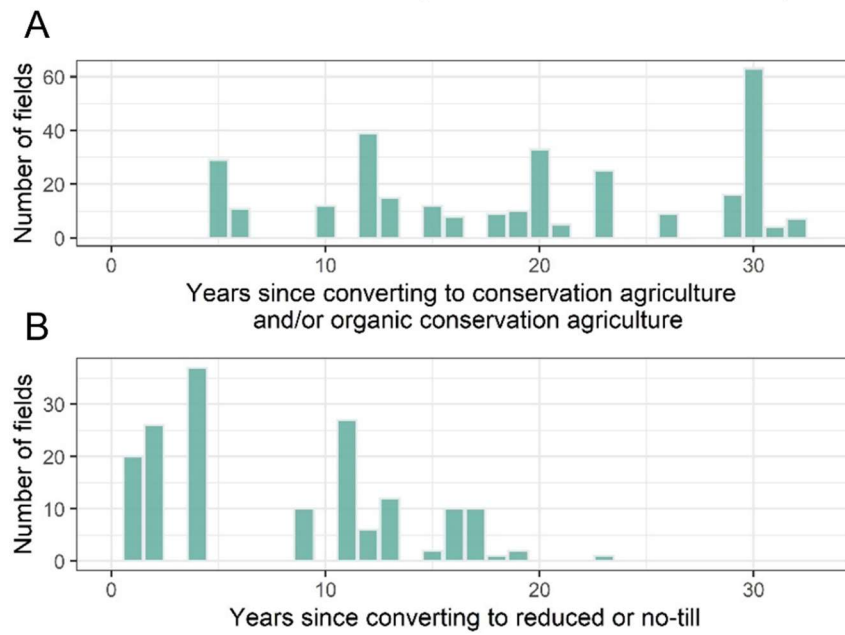


Figure 6.2: Years (counted from 2021) since (A) the conversion to conservation agriculture (CA) for the database containing 307 fields undergoing CA and (B) the conversion from conventional till to reduced or no-till for the 164 fields in carbon farming (CF) database. The 271 fields in CF where no tillage conversion was noted are not shown on the graph.

6.3.2 Matching

Before pursuing the matching, a correlation matrix was computed for quantitative control variables (Table A.6.1). A high correlation (absolute Pearson coefficient value > 0.8) was observed for the climatic control variables and elevation. Therefore, only two quantitative control variables were used to perform the matching procedure: clay and temperature, accompanied by the qualitative variable (agricultural region). The quality of the matching for each covariate was evaluated based on the standardized difference in means resulting from KS tests. Here, standardized difference was low (< 0.02) for all control variables. Two-sided KS test showed that the distributions

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of matched pairs for each covariate were equal (at 0.05 significance level; Figure 6.3). In total, as the matching operation dropped matched pairs that are too dissimilar, 286 control fields were matched to the CA database (307 treated fields), and 330 control fields were matched to the CF database (435 treated fields) (Table 6.3).

Table 6.3: *Number of fields in the two final databases after matching.*

Agricultural region	Conservation Agriculture		Carbon Farming	
	treated	control	treated	control
Sandy-loam	58	54	10	7
Loam	125	120	281	209
Condroz	90	86	108	91
Herbagère	11	6	-	-
Fagnes	15	13	-	-
Ardenne	-	-	23	13
Jurassic	8	7	13	10
<i>Total</i>	<i>307</i>	<i>286</i>	<i>435</i>	<i>330</i>

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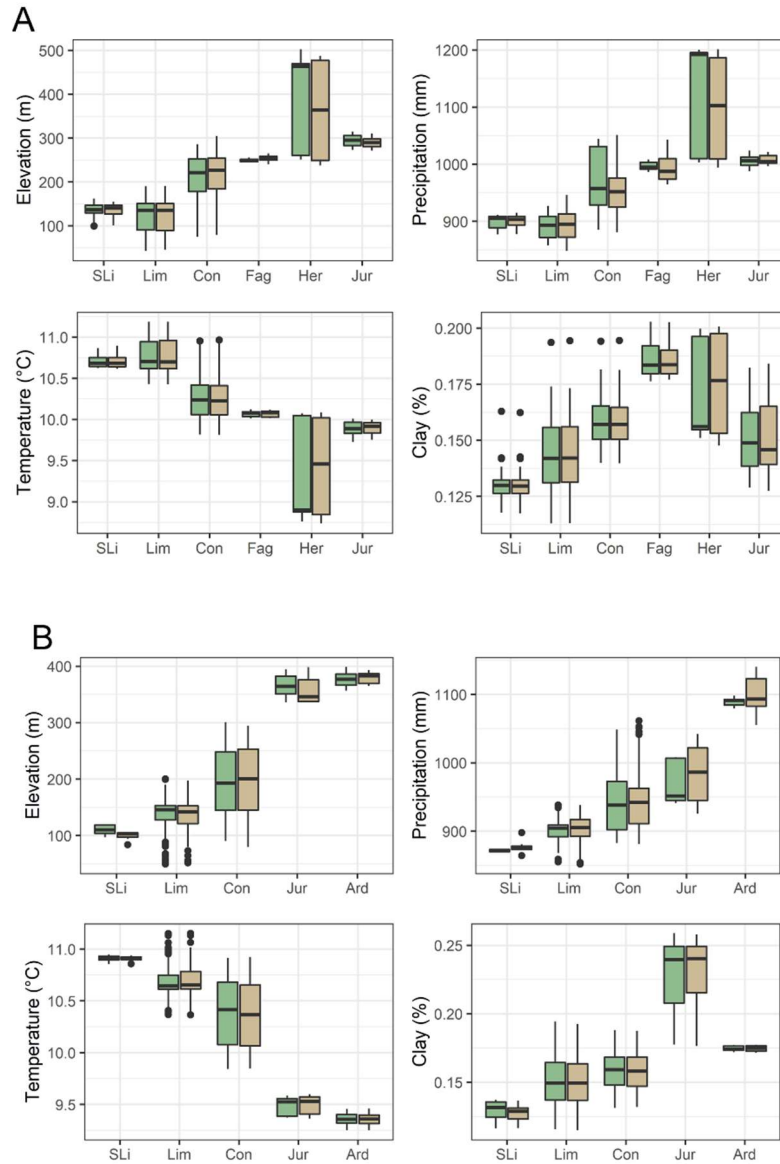


Figure 6.3: *The balance of covariates between matched pairs after performing nearest neighbor matching for (A) Conservation Agriculture (CA) database and (B) Carbon Farming (CF) database. In green are fields belonging to the CA or CF practices, in beige are the matched control fields with no presumed treatment.*

6.3.3 Spatial patterns

The key accomplishment of the SOC map produced from Sentinel-2 composite imagery in Chapter 5 is the ability to zoom in and visualize the difference in SOC content from one field to the other. Figure 6.4 shows an example of the SOC contents of two CA fields paired with a supposedly non-treatment field. Note that we cannot disclose the location for privacy reasons. The treated plots show a higher SOC content ($A = 14.4 \text{ g C kg}^{-1}$ and $B = 16.0 \text{ g C kg}^{-1}$) than the matched untreated plots ($A = 10.6 \text{ g C kg}^{-1}$ and $B = 10.9 \text{ g C kg}^{-1}$). However, the absolute difference (Equation 6.2) between the SOC content of treated and matched plots ($A = 3.8 \text{ g C kg}^{-1}$ and $B = 5.1 \text{ g C kg}^{-1}$) in both cases is lower than the detection limit (5.5 g C kg^{-1}) of the SOC map. Hence, based on the single mean value of SOC content predicted from a Sentinel-2 composite, no conclusion can be drawn about the effect of CA on SOC content in this example.

The bias of the SOC map was estimated at 0.5 g C kg^{-1} in Chapter 5, which was considered negligible. Moreover, the bias was estimated independently of any underlying field management condition. High-residue crop management and reduced- or no-till techniques are the key components of CA (FAO 2022). Fields under CA are therefore less exposed than fields under conventional agriculture. The spectral signature of crop residues affects the soil signal, resulting in a low degree of accuracy in soil mapping products (Hively et al. 2018). Additionally, we have shown that the uncertainty of SOC map increases when the number of scenes per pixel in a composite image decreases. It is therefore logical to assume that fields under CA with a higher residue cover and lesser soil exposure will suffer from a higher bias, compared to fields under conventional agriculture. Here, no difference in bias for CA and CF fields and conventional fields was acknowledged, for the following three reasons. Firstly, Normalized Burn

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ratio (NBR2) index was used to eliminate scenes with high moisture and residue cover. The resulting Sentinel-2 exposed soil composite is therefore free of the crop residue spectral signature. Secondly, in Chapter 5 we established that when at least six scenes per pixel are used, the uncertainty is minimized and does not further decrease. This threshold of minimum six scenes per pixel was respected when using the Sentinel-2 exposed soil composite derived SOC map in this work. Thirdly, in this study, tillage is considered as a technique that inverts soil horizons. Hence, non-inversion tillage (such as chisel or disk ploughing) which does not mix soil horizons is a no-tillage technique, and is still intensively used by CA farmers in Belgium. Soil surface in no-till CA or CF systems can therefore be still exposed, and can be included in Sentinel-2 exposed soil composite. Another limitation related to SOC mapping of CA/CF fields is the higher particulate organic matter (POM) associated with no- or reduced-till systems, related to higher concentration on residues (Six et al. 2001). Steffens et al. (2021) identified a higher absorption of the typical cellulose and lignin feature between 2000 and 2300 nm, related POM. This feature is located within S-2 B12, used in SOC prediction models.

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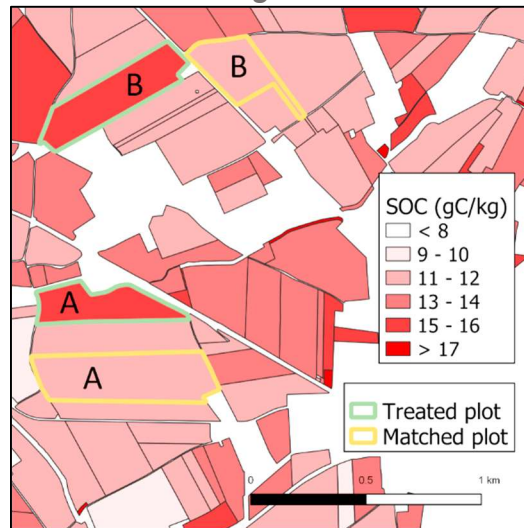


Figure 6.4: Zoom of the SOC per-field content modelled from Sentinel-2 composite (Chapter 5), and an example of two pairs A and B of treated (conservation agriculture) and matched plots in the Loam region of Belgium. For privacy reasons, the exact location of the fields cannot be disclosed.

6.3.4 Paired sites: regional analysis

A positive SOC gradient occurs from the northwest (Sandy-loam and Loam regions) to the south of Wallonia (Ardenne and Jurassic regions; Figure 6.5). This trend was previously described in the literature (Chartin et al. 2017; Meersmans et al. 2011) and is mainly correlated with the gradients in elevation, precipitation and temperature. SOC content in CA fields is on average higher than in control groups in all agricultural regions except for the Fagnes (Figure 6.5A). SOC content in CF is on average higher than in control groups in the Sandy-loam, Loam and Condroz regions (Figure 6.5B). The RR is significant for most regions demonstrating that the paired approach is able to detect differences in SOC content between CA/CF and conventional fields when regional averages of pairs are considered (Table 6.4). While RR between CA and CF are comparable in the Sandy-loam (18.8% for CA and 19.6% for

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CF) and Condroz regions (7.1% for CA and 5.7% for CF), CA practices show two times higher positive effect on SOC content (16.5 %) in the Loam region than CF practices (8.4%). When removing those CF fields in the Loam region that have switched towards reduced till less than five years ago, the RR of the leftover fields (81 fields) increased and became 17.9 %. For fields older than five years, RR was not significantly different between CA and CF databases (results not shown). The Jurassic region shows a large discrepancy in RR between CA and CF, where CA seems to have a highly positive effect on SOC content (RR = 27.1 %) and CF has a negative effect on SOC content in fields (RR = - 7.7%). Note, however, that the sample size in this region is very small (8 for CA and 13 for CF, Table 6.3). The RR for the entire datasets, without division into agricultural region, is 13.5% for CA and 6.4% for CF.

Derrouch et al. (2020) have shown that minimum five years are required for the farmer to master a new farming system, such as CA or CF. In the same context, Hobbs (2007) has estimated that soil physical and biological properties improve up to seven years after switching to conservation agriculture. This is in agreement with the major difference due to the selection criteria for the CA and CF databases. All CA farmers in the database have been practicing CA for more than five years, which is not the case for CF, where 50% of fields have switched to no- or reduced- till less than five years ago. We have shown that in the Loam belt, it is the inclusion of young fields in CF database that drops the RR.

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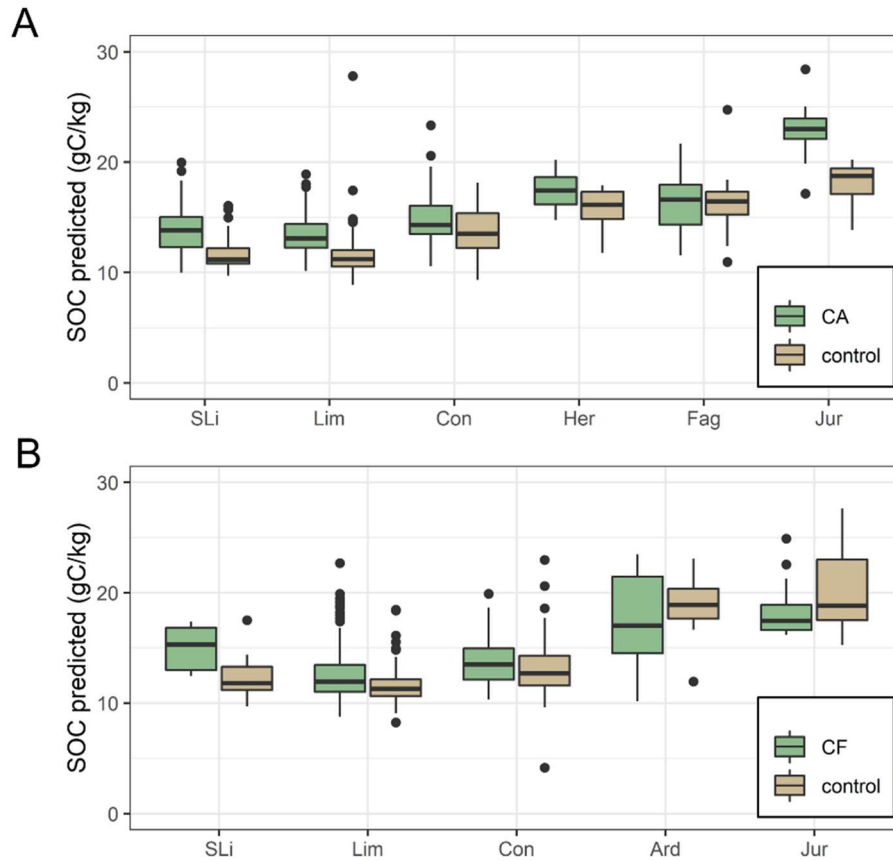


Figure 6.5: SOC values extracted from Sentinel-2 exposed soil composite SOC prediction (Chapter 5) for (A) the 307 conservation agriculture (CA) fields and the 286 matched control fields and (B) the 435 carbon farming (CF) fields and the 330 matched control fields per agricultural regions. SLi = Sandy-loam, Lim = Loam, Con = Condroz, Her = Herbagère, Fag = Fagnes, Ard = Ardenne and Jur = Jurassic. For the location of the agricultural regions, see Figure 6.1.

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Table 6.4: *Response Ratio* (Equation 6.1) for conservation agriculture (CA, $n=307$) and carbon farming (CF, $n=435$) databases and their matched fields where no special management practices are presumed.

Agricultural region	n		Mean Response Ratio (%)	
	CA	CF	CA	CF
Sandy-loam	54	7	18.8^a	19.6^a
Loam	120	209	16.5^a	8.4^b
Condroz	86	91	7.1^a	5.7^a
Herbagère	6	-	10.5	-
Fagnes	13	-	- 2.2	-
Ardenne	-	13	-	- 6.8
Jurassic	7	10	27.1^a	- 7.7 ^b

* *Bold numbers indicate that RR are significant at $\alpha=0.05$ between the treated and the non-treated fields. Same letters indicate no significant difference between CA and CF*

A second reason explaining lower RR for CF fields is linked to the carbon concentration effect in the upper soil in no- or reduced-till systems. A global meta-analysis carried out by Haddaway et al. (2017) has shown SOC stock increase in the upper soil layers (0-30 cm) in systems with no- or reduced- till, while no effect on SOC stocks was observed in the full soil profile. Higher SOC contents in the top soil promote a more productive soil with higher biological activity and provide resilience to extreme weather conditions (Haddaway et al. 2017), but no or little SOC sequestration is detected (Chenu et al. 2019). A non-negligible number of CF fields were still under conventional tillage (38%, Table 6.2), while this number was null for CA, as conventional tillage goes against the pillar 1 of CA practices (FAO 2022). Hence, the higher RR of CA might be due to the concentration of SOC in the topsoil due to the more frequent use of no or reduced-till.

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To our knowledge, matching based on spatial covariates has not been used yet with the aim to evaluate the effects of CF or CA practices. van Wesemael et al. (2019) tested the effects of management on the short to mid-term (5-10 years) SOC dynamics in long-term trials in agricultural soils of Wallonia. They found that fields in the Belgian Loam belt converted to conservation agriculture for at least ten years had more than 4 g C kg⁻¹ higher SOC contents than comparable fields under conventional agriculture. With the average SOC content in the topsoil (0-30cm) of the Belgian loam belt being 11.50 g C kg⁻¹ (Stevens et al. 2015), such an increase of 4 g C kg⁻¹ corresponds to an RR of 34.7% over ten years. We only observed RR's ranging from 8.4% for CF and 16.5 % for CA (both in the Loam belt, Table 6.4). Long term trials are carefully managed experiments, with controlled and long lasting treatments (Valkama et al. 2020). Such trials generally show larger effects than the one from management in farmers' fields, where treatments can evolve and variety of management options exist (Chenu et al. 2019). Here, we included fields under different management practices, with variable input of organic fertilizer, cover crop application, and mixed farming resulting in lower RR's than the ones from long-term trials (Table 6.2).

6.3.5 Paired site: field based analysis

6.3.5.1 The absolute difference approach

The absolute difference (Equation 6.2) was calculated for each matched pair (Figure 6.6). From 616 matched pairs, only 61 pairs (9.9%) had higher absolute difference than the detection limit set by the SOC map accuracy (5.5 g C kg⁻¹ at 95% confidence). 34 of the matched pairs with difference higher than the detection limit were from the CF database (10.3%), and 27 (9.4%) from the CA database. No trend was observed between the absolute difference and the duration since the conversion to no- or reduced- till (Figure 6.7). This result suggests that the Sentinel-2 composite-derived mean

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SOC map is not accurate enough to detect any changes in SOC which are due to CA or CF farming practices

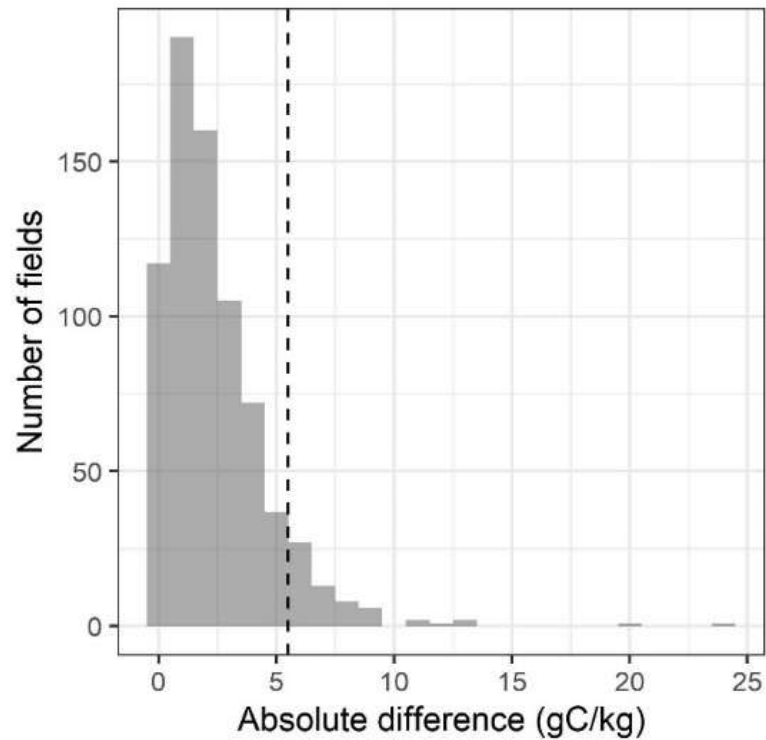


Figure 6.6: *Distribution of the absolute difference of SOC values (Equation 6.2) between treated and matched fields for each pair. The vertical dashed line represents the SOC detection limit of 5.5 g C kg⁻¹ at 95% confidence (Chapter 5). n = 616.*

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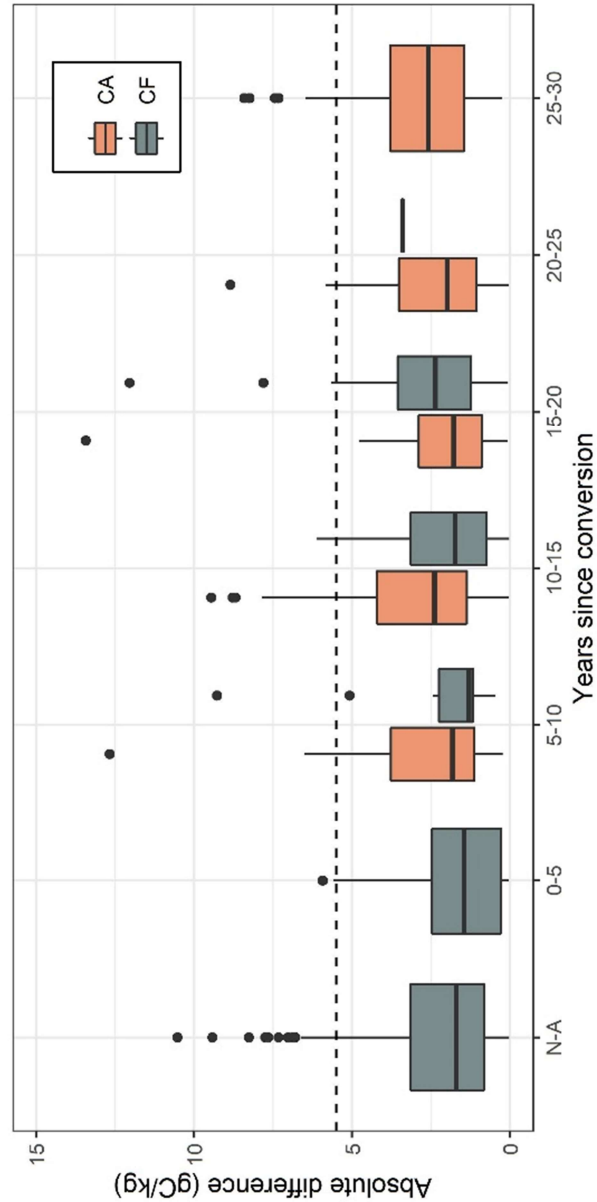
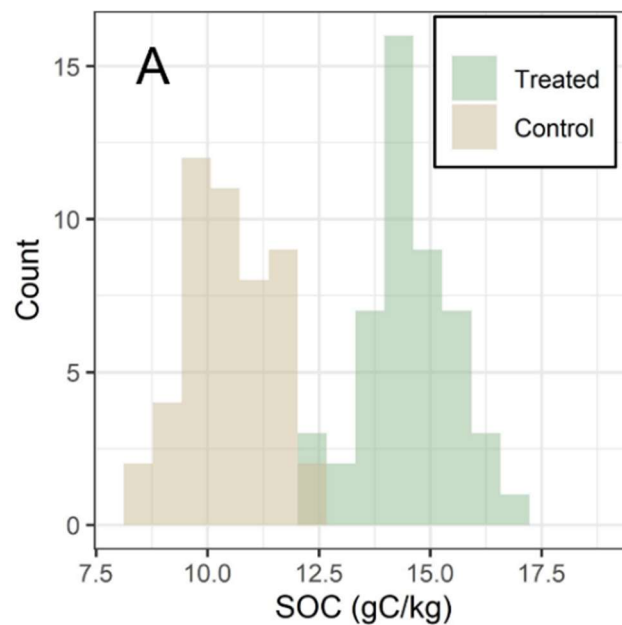


Figure 6.7: The absolute difference of SOC values (Equation 6.2) between treated and matched fields for each pair, in relation to the number of years since conversion to reduced or no-till. N-A group means that no conversion has taken place. CA = conservation agriculture ($n = 286$) and CF = carbon farming ($n = 330$). The horizontal dashed line represents the SOC detection limit of 5.5 g C kg^{-1} at 95% confidence (Chapter 5).

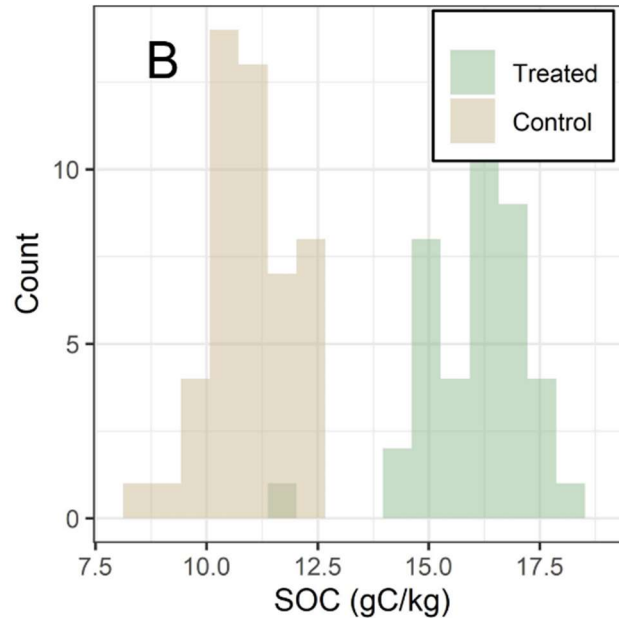
6.3.5.2 The bootstrapping approach

In order to deal with the small SOC changes to be expected, we exploited the potential of bootstrapping. Instead of one mean SOC value per field, 100 SOC predictions resulting from a bootstrapped model were available. An example of the two highlighted matched CA pairs Figure 6.4 is shown in Figure 6.8. While the absolute difference of the two pairs was smaller than the detection limit of the SOC map, the distribution of 100 SOC prediction resulting from bootstrapping clearly showed separate distributions of treated and control plots. Student's t-test test confirmed that the distributions of SOC content for treated and control groups were significantly different (at $\alpha = 0.05$ level) for these two pairs (Figure 6.8).



(A)

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(B)

Figure 6.8: *The distribution of 100 SOC predictions from 100-fold bootstrapping for an example of two pairs (A and B) of treated (conservation agriculture) and matched plots (see their location on the mean SOC map on Figure 6.4).*

The Student's t-test was carried out on all the matched pairs (286 for CA and 330 for CF) (Table 6.5). Pairs where either one or both distributions of SOC values did not follow the normality assumption were eliminated (Shapiro-Wilk). In total, 441 pairs (72%) followed a normal distribution (), and for 394 fields we detected a statistically significant difference (Table 6.5). Comparing population means of bootstrapping results therefore allowed to draw conclusion on the CA/CF effects on SOC content in fields for 72% of plots (441 put of 616 fields), compared to only 9.9% when relying on the model detection limit only. The exclusion of 28% of pairs because of the non-normality of their distributions can be solved by using a non-parametric

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equivalent of Student's t-test, for example the Kruskal-Wallis test which lacks the normality-assumption. However, since the use of non-parametric tests like Kruskal-Wallis is less preferred because they hold less power (Hecke 2012), parametric Student's t-test was used in this study. The percentage of fields where SOC content was higher than in the matched fields was greater for CA (72% for CA versus 65% for CF > 5 years and 46% for CF fields younger than 5 years, Table 6.5, Figure 6.9). Fields which have been converted to reduced or no-till in CF database more than five years ago show a higher success rate (Table 6.5, Figure 6.9) than fields that have been converted less than five years ago. This, again, confirms the findings of Hobbs (2007) and Derrouch et al. (2020) who both established that a starting period of at least five years is necessary before the effects of improved management reflects in the SOC contents.

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Table 6.5: Number of matched pairs in conservation agriculture (CA) and carbon farming (CF) databases after elimination of non-normal distributions or non-significant ANOVA analysis of SOC differences.

	CA (n = 286 matched pairs)	CF > 5 years (n = 330 matched pairs)	CF < 5 years	Total (n = 616)
Normal distribution for both treated and matched plots	169	48	224	441
SOC content in treated plot is higher than SOC content of matched plot	123 (72%)	31 (65%)	102 (46%)	256 (58%)

* Percentages are calculated based on the number of fields with normal distribution of SOC content

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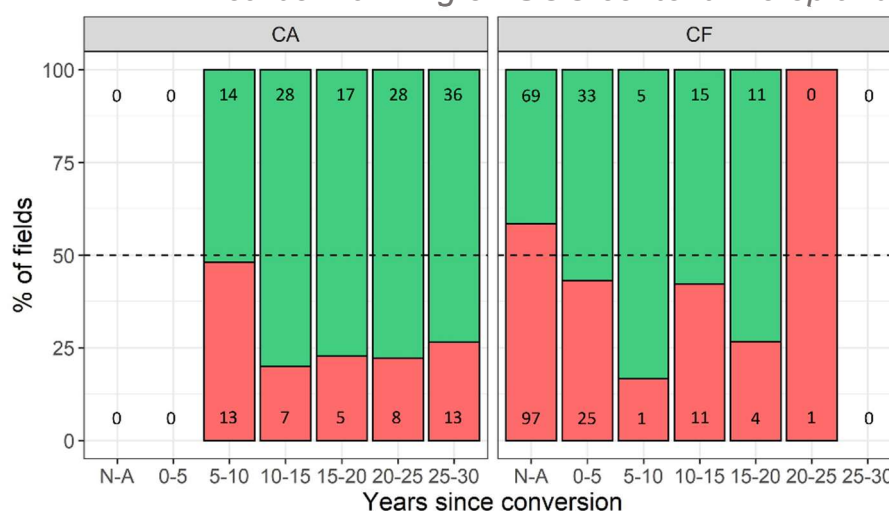


Figure 6.9: The percentage of fields where SOC content of treated fields (CA or CF) is greater (green) or lower (red) than the SOC content of matched fields. N-A group means for which no conversion has taken place. Number of pairs are indicated CA (n = 169) and CF = carbon farming (n= 272).

The Sentinel-2 exposed soil composite is a suitable tool for creating SOC maps at regional level, as we were able to detect significant response ratios (Table 6.4). However, a simple SOC map was inefficient to detect CA and CF effects on SOC content at a field scale, as the detection limit is high. To illustrate, Paustian et al. (2016) established that soil C sequestration rates on land maintained in agricultural use vary on the order of $0.1\text{--}1 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$, as a function of land-use history, soil or climate conditions, and the combination of management practices applied. In the best case scenario, $1 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$ equals to the increase of SOC content in the upper 0.3 m of agricultural soil of $0.27 \text{ g C kg}^{-1} \text{ yr}^{-1}$. Detecting such small SOC increase is unrealistic for an MRV system. Additionally, the diversity of CA and CF practices is very large, resulting in a high variability of SOC response (Giller et al. 2015). Giller et al. (2015) has stated that the reported beneficial effect of CA on SOC is

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inconsistent, and is secondary to CA. The primary effects of CA are the enhanced structural stability and the protection of the soil surface against erosion, reduced soil evaporation due to mulch cover, pest and disease control, biodiversity enhancement, and fuel saving due to reduced till (Giller et al. 2015). This can be a potential explanation to why some of the CA/CF fields showed no significant SOC increase. Hence, using SOC as an indicator for detecting fields under CA and CF does not seem as the best solution. However, at the scale of a region, we were able to detect increased SOC for fields under CA/CF compared to fields under conservation agriculture. Additionally, five-year compositing period was used to produce SOC maps. Therefore, as the effects of CA/CF on SOC can be observed after five years only, the minimum age of conversion to CA/CF should have been chosen as 10 years, allowing for a full five-year compositing period where SOC effects can be detected. This would however reduce the number of samples.

6.4 CONCLUSION

The frequency and high spatial resolution of freely available satellite imagery offer an unprecedented possibility to monitor space–time dynamics of SOC. The use of SOC products derived from remote sensing imagery are a reliable and cheap method to detect the effects of conservation agriculture and carbon farming on topsoil SOC content. At the scale of a region, the use of a response ratio has allowed to detect positive changes in SOC contents for fields under CA and CF. To detect SOC differences at the scale of a field, we have used the results of 100-fold bootstrapped model of SOC from a Sentinel-2 exposed soil composite in combination with statistical matching to find an appropriate baseline for comparison. This methodology detected a higher SOC content for 72% of fields under CA and 65% of fields under CF (for more than five years) compared to fields under conservation agriculture.

CHAPTER 7. GENERAL CONCLUSION

7.1 MAIN FINDINGS AND FOLLOW UP

The concern about the role of soils in the global carbon budget and the effects of SOC decline on soil quality has been incorporated in international treaties. Initiatives such as '4 per mille Soils for Food Security and Climate' or 'The Farm to Fork' strategy are being implemented in the context of Paris Agreement to mitigate climate change (Chapter 2). Implementation of such initiatives requires a robust, scientifically-sound measurement, reporting and verification (MRV) system to track that the policy goals are being met and that claimed increases in soil C stocks in croplands are real (Paustian et al. 2019). However, difficulties arise when implementing soil monitoring systems, as cost-effective and accurate SOC maps of croplands that cover large areas (regional/national), with high spatial (~20-50m) and temporal (5 years repeatability) resolution are needed. This thesis assesses the potential of remote sensing products to provide a tool for a rapid, repeatable, cost-effective and accurate monitoring for SOC content in croplands. This resulted in an original work as:

- We have tested different methodologies and state of the art concepts for pure soil pixels selection,
- We have validated NBR2 spectral index thresholds in the field in Wallonia,
- We have defined an improved methodology that allows to select pure soil pixels from Sentinel-2 imagery and derive a high accuracy SOC map including uncertainty map in Belgium, and

General Conclusion

- We have used S-2 derived SOC map and uncertainty map to evaluate the difference in SOC content of conservation agriculture and carbon farming fields from conventional agriculture fields, which has, to our knowledge, not been done before.

The conclusions are given according to the three different objectives presented in Chapter 1: (1) assessing the effects of disturbing factors on satellite derived SOC prediction, (2) creating S-2 exposed soil composite for SOC prediction in Wallonia and (3) testing the potential of the created SOC maps as a tool for detecting spatial changes in SOC content and distinguishing fields under conservation agriculture and carbon farming from conventional agriculture.

7.1.1 Assessing the effects of disturbing factors on SOC prediction

Soil spectra are very sensitive to dry residues left at the surface of the crops after tillage, and a meaningful calibration can only be done for smooth dry soil surfaces without residues. We have shown in Chapter 3 that when SOC prediction models are applied to a large area without prior knowledge of soil surface conditions, the disturbing effects of crop residues influence the SOC prediction accuracy. In particular, an overestimation of SOC has been observed for fields with extensive residue cover. It would be interesting to further evaluate the form of this overestimation (i.e. linear or exponential). Rodionov et al. (2016) established a non-linear relationship between CAI and SOC overestimation in croplands in laboratory conditions, but this finding should be upscales to airborne, or spaceborne, spectroscopy.

The removal of pixels with high residue cover on hyperspectral airborne image was proven to be feasible using a hyperspectral index based on the reflectance

around 200 and 2200 nm i.e. the cellulose absorption index (CAI), as shown previously (Chabrilat et al. 2011; Mzid et al. 2022). For dry soils in seedbed condition, the pure pixel selection based on CAI thresholds improved the SOC prediction accuracy. In particular, **we found that a CAI threshold of 0.75 allowed for the best SOC prediction model in the Loam belt**, which was not previously defined. This threshold was not tested outside of the Loam belt, and will likely vary with soil type, color and mineralogy. For multispectral satellite images, however, there was not yet a clear consensus on which spectral indices are suitable to eliminate spectra affected by crop residues. The potential of S-2 imagery for this purpose was investigated in the pilot zone of Belgian loam belt, and we found that **NBR2 index is suitable for selecting pixels with low crop residue cover**.

Additionally, we have demonstrated that when soils are dry and in seedbed condition, CAI and NBR2 indices based on both hyperspectral airborne and multispectral satellite sensors show a linear relationship. By extrapolation, a linear relationship exists between crop residue cover and both CAI and NBR2. However, we also found that **the linear relationship between NBR2 and crop residue cover does not hold when soils are wet**. We conclude that NBR2 is sensitive to soil moisture and can be used to detect moist soils when crop residues are not present.

7.1.2 Creating S-2 exposed soil composite for SOC prediction in Wallonia and Noord Holland

The removal of pixels affected by crop residues in Chapter 3 leads to a smaller soil surface exposure, as many pixels are masked out. Several authors have used composite images to increase the extent of the cropland area for which SOC content can be predicted (Castaldi 2021; Vaudour et al. 2021; Zepp et al. 2021). However, even the composites

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are hindered by the soil surface conditions, which might result in a decreased accuracy of SOC prediction models.

Therefore, **we have developed a methodology that allows creating S-2 exposed soil composites for SOC prediction by selecting S-2 pixels with minimal influence of the following disturbing factors: crop residues, surface crusts and soil moisture.** This was achieved in two ways. Firstly, by selecting the most suitable sensing period for extraction, as cultural operations have an impact on reflectance levels (Chapter 4). Secondly by gathering field observations and defining spectral index thresholds that allow to eliminate pixels with disturbing effects, independently of the crop calendar (Chapter 5).

In Chapter 4 we have explored the potential of pinning down the right acquisition date for each pixel based on the crop calendar. We defined as greening-up the instant for which the crop has been sown but has not yet emerged. This means that an eventual crust and crop residues have been ploughed in and soils are in seedbed condition (i.e. smooth). This is the closest we are able to get to the pure soil signal of the surface spectrum. Once the crop residues were removed by selecting the greening-up moment, we applied the NBR2 index in order to remove pixels with high moisture contents. **The SOC prediction models performed on composites built using the greening-up approach combined with NBR2 threshold performed well,** and actually outperformed any model applied to a composite which did not include the greening-up approach. However, the mappable area remains small (62% of croplands over a two year period). Additionally, the results suggested that even when using the greening-up approach, defining the correct spectral index threshold is important to obtain a correct SOC prediction.

Consequently, in Chapter 5 we gather field observations to define a methodology that allows masking out pixels affected by crusts, moisture, vegetation and crop residues,

independently of the cropping period. We have found that **applying an NBR2 < 0.05 threshold and normalizing the S-2 spectra allow obtaining a reasonable soil reflectance signal, where crop residues and moist soils are excluded, and crusts are corrected for**. Using these criteria in Google Earth engine, we built an exposed soil composite from Sentinel-2 imagery (covering the spring periods of 2016-2021), mapping 83% of croplands in Belgium and the Netherlands. The exposed soil composite was used to produce SOC prediction maps, accompanied by a measure of uncertainty. This compositing method showed both realistic within field and regional SOC patterns. **An accuracy of 5.5 g C kg⁻¹ was reached at the field level for 95% of samples.** The uncertainty of prediction was assessed via the PIR. On average, PIR represented 88% of the predicted SOC value. Such high uncertainty values render local SOC monitoring obsolete, however given the high accuracy of the SOC map, it may be a useful product to quantify average SOC at regional and national level.

7.1.3 Testing the potential of the created SOC maps as a tool for distinguishing the effect of CA and CF fields on SOC content

The high temporal frequency and high spatial resolution of satellite imagery offer an unprecedented possibility to study and monitor space–time dynamics of SOC change. In Chapter 6 we used the SOC map created in Chapter 5 and tested its potential to distinguish the effects of conservation agriculture (CA) and carbon farming (CF) on SOC content. We have used the results of 100-fold bootstrapped model of SOC from Sentinel-2 exposed soil composite in combination with statistical matching to find an appropriate baseline for comparison. This methodology showed that for **72 % of the CA pairs and 65% of the CF pairs a significant difference in SOC content exists between fields under CA and CF compared to fields with no treatment.** By

using the large quantity of data available from remote sensing, we were able to bypass the issue of low accuracy of remote sensing data.

7.2 PERSPECTIVES

The removal of pixels with disturbing effects from multispectral satellite images is a key to success of SOC prediction models. Especially the removal of crop residues allows improving SOC prediction models (Chapter 3). In Chapter 5 we have shown that the SWIR region is the one most affected by crop residues and moisture content. Removal of affected pixels however still remains particularly challenging, due to the low spectral resolution of S-2 MSI in the SWIR region. S2 has only two SWIR bands poorly situated to capture the narrow lignin-cellulose spectral absorption features (Hively et al. 2021). Currently, there are hyperspectral satellite data sources such as PRISMA and EnMap that provide imagery with sufficient SWIR coverage to map crop residues at a regional scale (Hively et al. 2021). However, they do not have the desired temporal and spatial coverage like a multispectral mission to provide a sufficient volume of data. Hively et al. (2021) proposed additional spectral bands for the Landsat 9 follow-on mission, Landsat Next, expected to be launched in the late 2020s. They argue that bands centered at 2040, 2100, 2210 and 2260 nm with 30 nm bandwidth should be added for measurement of ligno-cellulose absorption features to support detection of crop residues, while avoiding spectral regions prone to atmospheric disturbance.

However, considering the rising popularity of conservation agriculture, SOC mapping from remote sensing might become all the more challenging. If croplands are continuously under crop residue cover, the selection of pure soil pixels will significantly reduce the exposed area to be mapped. Hence, unmixing might have to be applied, to decompose image pixels into bare soil and its other

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constituents, the endmembers. Using multispectral satellite imagery for spectral unmixing is however challenging (Laamrani et al. 2020; Pacheco and McNairn 2010), and the use of hyperspectral data is preferred (Asner and Heidebrecht 2002). So far, spaceborne hyperspectral data are available at limited scale from missions including Hyperion, TianGong-1, PRISMA, HISUI, EnMAP, Shalom, EMIT, and HypXIM (Transon et al. 2018). The planned launch of Copernicus Hyperspectral Imaging Mission for the Environment (CHIME) as a complement to the S-2 mission could be a game changer, as it provides large spatial coverage for land-cover mapping.

The use of mobile phone georeferenced RGB images of crop residues could constitute an interesting follow up to our work. d'Andrimont et al. (2018) illustrated the huge potential of crowdsourcing, or *citizen science*, as a complementary sampling tool. A large quantity of RGB photographs of field conditions could expand the database available for soil surface conditions classification. Such large amount of information could (1) be used to define thresholds locally, allowing for a better SOC model quality, and (2) constitute a spectral library for unmixing purposes. The hyperspectral simulation of canopy reflectance system (HySimCaR), which is a spectral, spatial and temporal simulation system that can model detailed virtual cereal canopies of different phenological stages, is currently used to simulate the spectral information of various soil types with fractional green and dry vegetation cover (Kuester et al. 2014). While it constitutes a helpful tool for simulating the effects of mixed signals, it is not suitable for applications over large areas. Hence, the crowdsourced RGB phone images could be a suitable alternative.

Given the freely available satellite imagery, the largest cost associated to SOC mapping from remote sensing lies in the soil sampling. This can be fixed through the establishment of spectral libraries, which contain both spectral measurement and corresponding soil properties, measured

with reference methods of soil analysis (Nocita et al. 2013). Not only does centralized spectral library set the precise conditions of measurement, it also allows a greater variation in a training set, which increases the ability of the statistical models to predict SOC (Stevens 2008). Several spectral libraries are freely available, e.g. the ICRAF-ISRIC world soil spectral library (4 438 soil samples) or the European spectral library LUCAS (20 000 topsoil samples). Several studies have shown the potential of spectral libraries for large scale SOC mapping using simulated spaceborne data (e.g. Tziolas et al. (2020), Ward et al. (2020)), however there are several issues intrinsic to the use of global spectral libraries for SOC model calibration and validation, and specific methodologies need to be developed, among others local spectral libraries.

7.2.1 Remote sensing for MRV?

COWI (2021) stated that two factors are central to determining whether a cost-effective result-based MRV scheme is feasible: (i) the ease and degree of certainty with which the results can be measured, and (ii) the degree of risk to which the result-based approach exposes the farmer. The following two paragraphs will address these factors.

Firstly, the key challenge in all result-based schemes is designing an MRV system that is sufficiently accurate at an acceptable cost to both the farmers and the administrators (COWI 2021). There is a trade-off between the accuracy of the indicator measurement and cost, and reducing uncertainty is likely to increase costs (financial and time) (COWI 2021). High costs reduce the voluntary farmer uptake and the overall impact of the scheme (COWI 2021). Hence, the key strategy is to keep costs low enough to encourage widespread participation, whilst ensuring sufficient monitoring accuracy. To limit the costs of a monitoring system, we tested the use of Sentinel-2 derived SOC maps for monitoring the impacts of CA and CF

participants. **Using freely available Sentinel-2 data and a limited number of local soil samples (124 samples), we have mapped 65% of croplands in Wallonia (Chapter 5). This has allowed us to detect higher SOC content in 72% of CA fields and in 65% of CF fields (Chapter 6).** This illustrates the advantage of remote sensing for soil property mapping at large scales. **While the product accuracy is lower than for in-situ measurement techniques, the large amount of data and the high possibility for repeatability overshadows the low accuracy issue.**

Secondly, the issue of farmers' risk exposure needs to be addressed. An unfair MRV increases the chances of non-delivery to the farmers. A non-negligible percentage of fields were eliminated due to external factors outside of farmer's control, and could therefore not be a part of the MRV scheme. Hence arises the question whether it is possible to apply an MRV scheme where some potential users are excluded due to no fault of their own.

An additional limitation to our approach is the use of SOC content, and not SOC stocks, as indicator. The bulk density, vertical gradient in SOC content and the stone content are additional variables necessary for SOC stock calculation, but are not provided by the spectroscopic approach used in this thesis. Especially soil bulk density is a difficult parameter to measure accurately in field by proximal sensing (Bellon-Maurel and McBratney 2011). Satellite imagery SOC products can however be used as covariates in digital soil mapping which predict SOC stocks using point observations and satellite imagery (McBratney et al. 2003). Including a vertical SOC gradient will correct the issue of SOC concentration at the soil surface in no- or reduced- till systems.

Overall, SOC map derived from Sentinel-2 exposed soil composite has shown to be a potential starting point for a regional soil monitoring scheme, but by itself, the product is

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unable to deliver SOC stock monitoring system yet. It is however worth investigating whether including the Sentinel-2 SOC map as a covariate in digital soil mapping techniques as suggested by Smith et al. (2020) could lead to a fully functioning result-based MRV scheme.

APPENDIX

APPENDIX 1 (CHAPTER 3)

Table A.3.1. *Descriptive statistics of the SOC calibration dataset and the results of the Partial Least Squares Regression (PLSR) model per various spectral pre-treatments. R = Reflectance, A = Absorbance, SG = Savitzky–Golay smoothing, FD = 1st derivative, SD = 2nd derivative, SNV = standard normal variate, CR = continuum removal. In bold is the pre-treatment which provides the best model.*

Treatment	LV	RMSE *	R ²	RPD
Reflectance	7	2.40	0.38	1.24
Absorbance	13	2.14	0.49	1.39
SG-R	7	2.42	0.36	1.23
SG-A	9	2.33	0.40	1.28
FD	7	2.26	0.44	1.32
SG-FD	12	2.36	0.39	1.26
SD	9	2.80	0.24	1.06
SG-SD	12	2.31	0.41	1.28
SNV	5	2.45	0.33	1.21
SNV detrend	4	2.40	0.36	1.24
CR	6	2.29	0.42	1.29

* expressed in g kg⁻¹.

Table A.3.2. *p*-value of Levene's test of homogeneity of variances between training sets of various CAI thresholds. Null hypothesis: the population variances are equal. In bold: training set combinations that reject the null hypothesis at $\alpha = 0.05$ and whose variances are therefore not equal.

[illegible]

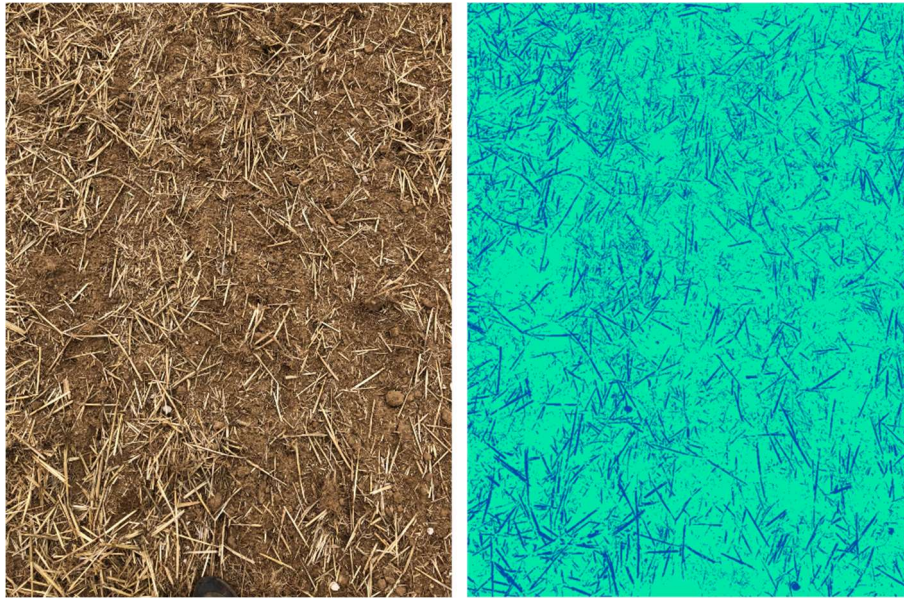


Figure A.3.1: iPhone RGB image of the Sicy field taken on 02-09-2018 (left), and the result of maximum likelihood supervised image classification performed in ArcGis (right). The residues are in blue, and cover 24% of the soil (green).

APPENDIX 2 (CHAPTER 4)

Table A.4.1. *p*-value of Levene's test of homogeneity of variances between training calibration datasets for the various composites. Null hypothesis: the population variances are equal. In bold: Training set combinations that reject the null hypothesis at $\alpha=0.05$ and the variances of which are therefore not equal. For interpretation of the composites see Table 4.2.

Composite									
	A	B	C	D	E	F	G	H	I
A									
B	0.890 0.114 0.048								
C	0.390 0.332 0.666 1.000	1.000							
D	0.890 0.114 0.048	0.390 0.332 0.666 1.000	-						
E	0.890 0.114 0.048	0.390 0.332 0.666	1.000						
F	0.890 0.114 0.048	0.390 0.332 0.666	1.000	-					
G	0.705 0.193 0.098 0.641 0.592	-							
H	0.495 0.338 0.207 0.979	-							
I	0.495 0.339 0.278	-							
	0.117 0.881	-							
	0.141	-							
	-								

APPENDIX 3 (CHAPTER 5)



Figure A.5.1: General flowchart for creating composites for assessing the link between uncertainty and number of scenes per pixel.

APPENDIX 4 (CHAPTER 6)

Table A.6.1. Correlation coefficients between the different environmental covariates

	Clay	Precipitation	Elevation	Temperature
Clay	1.00	0.42	0.42	-0.43
Precipitation		1.00	0.93	-0.93
Elevation			1.00	-0.99
Temperature				1.00

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