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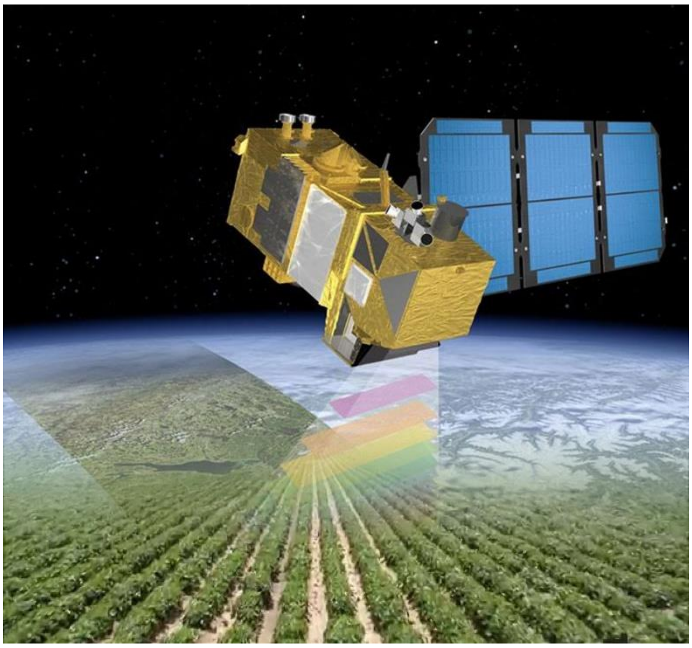
Estimating leaf chlorophyll of a potato crop using radiative transfer modelling and vegetation indices in precision agriculture

Niek Fischer



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Estimating leaf chlorophyll of a potato crop using radiative transfer modelling and vegetation indices in precision agriculture

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IV. Foreword

This thesis was inspired by the impressive technological advances made on the Van De Borne potato fields, who believes in the advantages of precision agriculture for productivity and environment. Working on this research was based on a personal interest of automating and monitoring many processes in agriculture in real time. A special thanks goes out to J. Verrelst for providing the software package ARTMO and giving support to keep ARTMO up to the needs of this study. Hopefully this study adds to the potential of ARTMO and making it more popular in the remote sensing community. Another thanks goes out to B. Kooij for creating the front image.

V. Abstract

The estimation of leaf chlorophyll using canopy spectra with combined radiative transfer modelling and vegetation indices has not been researched intensively. However, estimation of leaf chlorophyll using spaceborne sensors (Sentinel-2 & VENµS) could provide interesting applications in precision agriculture. The aim of this research was to estimate leaf chlorophyll content of a potato crop using radiative transfer modelling and vegetation indices on simulated bands of two spaceborne sensors and CropScan spectral measurements. The vegetation indices used were: NDVI, CVI and TCARI/OSAVI. Firstly a sensitivity analysis was performed using PROSAIL and the vegetation indices. Secondly, the models were improved where possible using: Best Band Combination and model constraint. Thirdly, simple regression was performed on the outcome of the PROSAIL models. Finally, these regressions were validated on spectral field measurements of a potato field. Important outcomes of this research are: 1) the model that performed most optimal was the PROSAIL model based on TCARI/OSAVI after a model constraint improvement limiting the range of possible leaf angles for potatoes. 2) A ratio index using Sentinel-2 bands at 705nm and 1375nm, resembling the NDWI, was found to also be able to perform leaf chlorophyll estimation from canopy spectra.

1. Introduction

1.1. Precision Agriculture

Precision farming is since the 1990's an upcoming and popular new way of thinking about agriculture (Mulla, 2013), where more focus is laid upon sustainability and quality of the environment. Precision agriculture is a production system that promotes variable management practices within a field, according to site conditions (Seelan, Laguette, Casady, & Seielstad, 2003). Many precision agriculture techniques and benefits are described in a review by Mulla (2013). Remote Sensing is a promising tool in precision agriculture as it is a non-destructive method of monitoring vegetation. Generally, remote sensing in precision agriculture uses two approaches; a physical and a statistical approach. The physical approach encompasses radiative transfer modelling using large models and parameterizing vegetation characteristics (Dawson, Curran, & Plummer, 1998; Jacquemoud & Baret, 1990; Jacquemoud et al., 2009). The statistical approach involves the creation of statistical models based on the spectral data itself. These statistical models can be based on spectral reflectance and vegetation index values. Vegetation indices play an important role at interpreting satellite data, these relate spectral information to vegetation properties. Usually used statistical models here are Simple Regression (Liu, Pattey, & Jégo, 2012; Magney, Eitel, Huggins, & Vierling, 2016), Multivariate Regression (Arenas-Garcia & Camps-Valls, 2008; Hansen & Schjoerring, 2003; Lausch et al., 2013) and Machine Learning Algorithms (Omer, Mutanga, Abdel-Rahman, & Adam, 2016) . The approaches are used for the simulation and prediction of vegetation properties. Precision agriculture continuously aims to become more and more accurate using increasingly sophisticated sensors, large and detailed databases and better methodologies, such as improvements to previously mentioned approaches. An overview of technologies and trends in precision agriculture are described by Zhang, Wang & Wang (2002). Advances in precision agriculture have also led to an increase in performance of data collection (sensors, computing power, etc.). With these advances there is a transition from measuring crops in the field to measuring a crop in a field. Most models used to create crop predictions are based on canopy chlorophyll, where one would look at a whole field. Now, with current advancements a single crop can be assessed using leaf chlorophyll as a parameter for modelling. This increase in accuracy improves estimations in the plant nutrient balance, disease recognition, weed infestations (Thorp & Tian, 2004). An improvement to the current physical approach is increasing the precision of radiative transfer models by using leaf chlorophyll instead of canopy chlorophyll.

1.2. Radiative transfer models

With the use of radiative transfer models one tries to model reality and estimate certain parameters which can be related to vegetation indices. In this particular research PROSPECT-5 (Feret et al., 2008) and 4SAIL (Verhoef & Bach, 2007) are used. Both models are operationally used in precision agriculture. PROSPECT-5 is a radiative transfer model which is focused on the leaf level. PROSPECT-5 is based on PROSPECT; a model of leaf optical properties spectra (Jacquemoud & Baret, 1990). PROSPECT-5 is an improved version in which chlorophyll is separated from the carotenoids. 4SAIL (Verhoef, Jia, Xiao, & Su, 2007) is an improved version of the SAIL (Scattering by Arbitrary Inclined Leaves) model (Verhoef, 1984). 4SAIL is a more numerical robust and speed optimized version of SAIL. It is also a radiative transfer model, but is based on canopy properties. There are numerous other variations and combinations, but these will not be used for this research. These two radiative transfer models are later on combined into PROSAIL (Verhoef, 2005). PROSAIL is currently the most popular radiative transfer model used in remote sensing (Jacquemoud et al., 2009). The model is designed to describe both spectral and directional variation of canopy reflectance as a function of leaf biochemistry and canopy structure.

1.3. Vegetation indices

Vegetation indices play an important role at interpreting satellite data, these relate spectral information to vegetation properties. Indices are calculated as ratios or as differences of several bands in the spectral regions: Visible spectrum (VIS), Near Infrared (NIR) and Shortwave Infrared (SWIR). Their applicability relies on its high correlation with biophysical parameters of plants (Wojtowicz, Wojtowics, & Piekarczyk, 2015) and low sensitivity to factors that make remote sensing data interpretation difficult, such as: atmosphere, soil background, viewing angle and non-green elements of vegetation (Huete, Justice, & Leeuwen, 1999). The Normalized Difference Vegetation Index (NDVI) has very common use in remote sensing (Rouse Jr, Haas, Schell, & Deering, 1974). This index is a ratio vegetation index, that calculates the difference and the sum of the red and NIR spectral regions, followed by the quotient of this difference and sum. A potential interesting vegetation index for leaf chlorophyll estimation, which is more focused on crops is the Transformed Chlorophyll Absorption in Reflectance Index (TCARI) divided by the Optimized Soil-Adjusted Vegetation Index (OSAVI). The index is based on the theory that leaf chlorophyll can be calculated by dividing canopy chlorophyll by the Leaf Area Index (LAI). TCARI is an index which is sensitive to canopy chlorophyll and

OSAVI is sensitive to LAI and insensitive to soil background. TCARI/OSAVI is sensitive at low LAI, minimizes the soil background effect and is resistant to solar angle variations (Haboudane, Miller, Tremblay, Zarco-Tejada, & Dextraze, 2002). An especially interesting band configuration to predict crop chlorophyll with TCARI/OSAVI is centered at 705nm and 740nm for Sentinel-2 (Clevers & Gitelson, 2013). Another interesting index is the Chlorophyll Vegetation Index (CVI) (Vincini, Frazzi, & D'Alessio, 2007). The CVI is developed specifically to predict leaf chlorophyll content and works well with planophile crops. CVI outperformed on canopy scale level as a predictor for leaf chlorophyll (Vincini, Amaducci, & Frazzi, 2014).

1.4. Canopy chlorophyll to leaf chlorophyll

There is a need to find better correlations between vegetation indices and vegetation properties, which could lead to better productivity estimations for environmental and agricultural applications (Herrmann et al., 2011). From a remote sensing perspective vegetation research is usually done at canopy level, because imagery is not detailed enough to measure at leaf level (Yoder & Pettigrew-Crosby, 1995). In precision agriculture it becomes more interesting to look at these slight variations in leaf chlorophyll to obtain a better understanding of the processes in individual plants. Canopy chlorophyll content is determined by the LAI and the leaf chlorophyll content (LCC) (Gitelson, 2005; Kooistra & Clevers, 2016). Current satellite image pixel sizes are still rather large for precision agriculture. Upcoming satellites like Sentinel 2 (10m) and VENμS (5.3m) have much better spatial resolution and have a larger potential for precision agriculture than for example Landsat 8 (30m). The transition from canopy reflectance spectra to leaf reflectance spectra is very complicated, because of variations in background reflectance and LAI confounded detection of very subtle differences in canopy reflectance due to changes in leaf chlorophyll concentration (Daughtry, 2000). Leaf chlorophyll is often measured using a handheld device called SPAD. Correlation between SPAD measurements and leaf chlorophyll have been found in the field (Jongschaap & Booij, 2004). The large scale difference between remote sensors measuring canopy chlorophyll and handheld sensors measuring leaf chlorophyll has caused that much research has been done on canopy chlorophyll content with remote sensing (Clevers & Gitelson, 2013; Clevers & Kooistra, 2014; Gitelson, 2005; Haboudane et al., 2002; Herrmann et al., 2011; Houborg et al., 2015; Nguy-Robertson et al., 2014; Vincini et al., 2007; Vincini, Frazzi, & D'Alessio, 2008), but there is much less research done on leaf chlorophyll content (Cohen et al., 2010; Vincini et al., 2014; Vincini & Frazzi, 2009, 2011).

1.5. Objective

The objectives for this research are to find a relation between remote sensing observations and leaf chlorophyll content. To achieve this I will investigate which potential vegetation indices are most applicable to potato crops. Many methods used are revolving around either crop chlorophyll or leaf chlorophyll. This study will assess which method will best predict leaf chlorophyll contents. A software program (ARTMO) will be explored, which is adapted to performing calculations and simulations with spectral information, and to which extent this can aid the research. For application purposes it is interesting to compare two specific space borne sensors, because they have slightly different band configurations. To formulate these into research questions:

- Which vegetation indices are most suitable for predicting leaf chlorophyll content as obtained from a sensitivity analysis using radiative transfer models in ARTMO?
- What is the effect of spectral band definitions and different sensors on the selected vegetation indices and on their relationship with leaf chlorophyll content?
- How can predictive models from radiative transfer modelling and validated on field measurements be improved to increase their accuracy?

2. Materials & Methods

2.1. Materials

2.1.1. Van De Borne dataset (VDB)

All data important to this study were collected at the Van De Borne (VDB) potato fields (Clevers & Kooistra, 2012). The VDB fields were located in the South of the Netherlands. Several plots were laid out there, of 30 by 30 meters, containing different nitrogen-containing fertilizer amounts and forms (Clevers & Kooistra, 2014). Spectroradiometric data was gathered using the CropScan Multispectral Radiometer (MSR16R); this sensor is referred to CropScan further along. It measured incoming and reflected radiation in 16 narrow spectral bands (Appendix Table 9). Calibration was performed by pointing the 28˚ FOV aperture towards the sun using an opal glass. Using this calibration, spectral reflectances were derived. The dataset included data on LAI, SPAD measurements (Vos & Bom, 1993) and spectral information from CropScan. SPAD data were converted to leaf chlorophyll with a potato specific model by Uddling (2007). From the dataset everything else that was needed could be easily calculated. The measurements were taken in the years 2010, 2011, 2012 and 2013.

2.1.2. ARTMO

The radiative transfer models and vegetation indices were collected in a program called Automated Radiative Transfer Models Operator (ARTMO) (Verrelst, Romijn, & Kooistra, 2012). Its purpose was a collection of analysis methods for leaf and canopy models and spectral indices and functions as a toolbox. ARTMO let one very simply add new spectral indices which could be immediately translated to all sensors available, because it read the spectral band into the equation of the index introduced into ARTMO. Furthermore, it included several tools to support this analysis. This program was used because its purpose fits into the methods that were used. It was also very capable of doing sensitivity analysis due to its fast computing power, which ensures that a large number of parameters can be varied. This improved the sensitivity analysis.

2.1.3. PROSAIL

In the analysis the most relevant properties included in the radiative transfer models PROSPECT-5 and 4SAIL were varied within ARTMO. According to literature, these were LAI and leaf chlorophyll. The results from the PROSPECT-5 model were implemented in the

4SAIL model, which would therefore be a PROSAIL analysis. The step size to simulate a spectrum was defined by the spectral band of the sensors as described in Table 10 & Table 11 of the Appendix. A step size of 1nm was possible, however, this would produce 378,180 simulations with the variables presented below (Table 1). Therefore, it was chosen to only use the wavelengths given by the sensors' configuration, which was supported by the objective to search for any differences between sensors.

Table 1: Overview of parameters inputted in ARTMO used to create PROSAIL simulations

PROSAIL parameters	**Nominal values**
Leaf structure parameter (N)	1.5, 2.0, 2.5
Chlorophyll concentration (C_{ab})	5, 10, 15, 20, 30, 40, 50, 60, 70, 80 µg/cm^2
Carotenoids	7 µg/cm^2
Brown Pigments	0
Water thickness (C_w)	0.0137 g/cm^2
Dry matter (C_m)	0.010 g/cm^2
Leaf Area Index (LAI)	0.5, 1.0, 1.5, 2, 3, 4, 5, 6
Hot spot effect	0
Leaf Angle Distribution (LAD)	0°, 45°, 90°
Solar zenith angle	30°, 45°, 60°
Diffuse/Direct radiation	0
Soil coefficient	0
Sun-view Azimuth angle	0°

In Table 1 the different parameters are shown that were used for sensitivity analysis in PROSAIL. Leaf chlorophyll content was the most important variable in the analysis so this content had the largest number of steps. Carotenoids had a constant value, this was because around a wavelength of around 560nm its absorption coefficient value approaches zero, meaning that the effect of carotenoids from R_{GREEN} onwards was very low. Brown pigments were kept at zero because a completely green plant was assumed. LAI was according to most literature a very important variable which explains the variation in canopy chlorophyll in a model. Leaf structure could be of interest for plants such as potato plants. Potato plants grow with a different leaf orientation throughout the season, this could potentially give interesting results regarding LAD and solar zenith angle. Rather extreme values of LAD were assumed, this was to assess how the models behaved under this extremity. C_w and C_m were values commonly used for potato crop simulations. Besides the LAI, LAD and solar zenith angle the other 4SAIL parameters were kept constant, so that the effects of the more important parameters during sensitivity analysis were observed better.

2.1.4. Satellite systems (Sentinel-2, VENµS)

Sentinel-2 and VENµS (Vegetation and Environment monitoring on a New Micro- Satellite) are two satellites which missions include monitoring of land systems such as agriculture and natural areas. Both contain multiple bands in the Visible (VIS) and Near InfraRed (NIR) wavelength regions. The design of the Sentinel-2 mission aimed at an operational multi-spectral Earth-observation system that complemented the Land-sat and SPOT (Satellite Pour l'Observation de la Terre) observations and improved data availability for users (Drusch et al., 2012). Sentinel-2 was launched on June 15th 2015. It contains 13 bands of which 10 bands would be highly applicable for use in vegetation indices. These 10 bands are situated in the VIS and NIR regions (Appendix Table 10). It has a swath width of 290km by applying a total FOV of about 20˚. VENµS scientific objective is the provision of data for scientific studies dealing with the monitoring, analysis, and modelling of land surface functioning under the influences of environmental factors as well as human activities (Centre National d'Etudes Spatiales (CNES)). VENµS will be launched in June 2017. It contains 12 high spatial (5 to 10 meter) and temporal (2 days) resolution bands. All bands of this sensor will be applicable on vegetation analysis and can be implemented in vegetation indices (Appendix Table 11).

2.1.5. Vegetation indices

A detailed overview of the vegetation indices described in Section 1.3 is given in Table 2.

Table 2: Overview of vegetation indices used, with formulation

Index	**Formulation**	**Reference**
CVI	$CVI = \frac{NIR * RED}{GREEN^2}$	(Vincini et al., 2007)
NDVI	$NDVI = \frac{NIR - VIS}{NIR + VIS}$	(Jackson, 1983)
TCARI/OSAVI	${TCARI}/{OSAVI} = \frac{3[(R_{700} - R_{670}) - 0.2(R_{700} - R_{550})\left({R_{700}}/{R_{670}}\right)]}{(1 + 0.16)\,{(R_{800} - R_{670})}/{(R_{800} + R_{670} + 0.16)}}$	(Haboudane et al., 2002)

Further along the report there will be more references to these indices concerning their position within the equation. Therefore, within CVI the position in the bands of: GREEN, RED and NIR would be referred to as R_{GREEN}, R_{RED} and R_{NIR} respectively. The same concept applied to NDVI where: VIS and NIR are referred to R_{RED} and R_{NIR} respectively. R stood for the reflection in a spectral band, R_{GREEN} was therefore the reflection in a band of a sensor chosen to be on the position of GREEN within the CVI. TCARI/OSAVI was already defined using R for the reflectance in a spectral band. This definition was chosen, because the spectral bands were chosen by Haboudane et al. (2002) as such. If these spectral band choices were presented more 'freely', such as NDVI, this would have large effects on further analysis in this study. Analysis of TCARI/OSAVI would be impossible, because the theory behind these specific bands would be neglected.

2.1.6. Process

Figure 1 shows the flowchart illustrating the order of processes which are further described in Section 2.2. As shown below the vegetation indices (Section 2.1.5) and PROSAIL parameters (Section 2.1.3) were used in the sensitivity analysis (Section 2.2.1). Here a choice was made to improve (Section 2.2.2) or not, followed by the estimation of leaf chlorophyll content which was validated (Section 2.2.3) on the VDB dataset (Section 2.1.1).

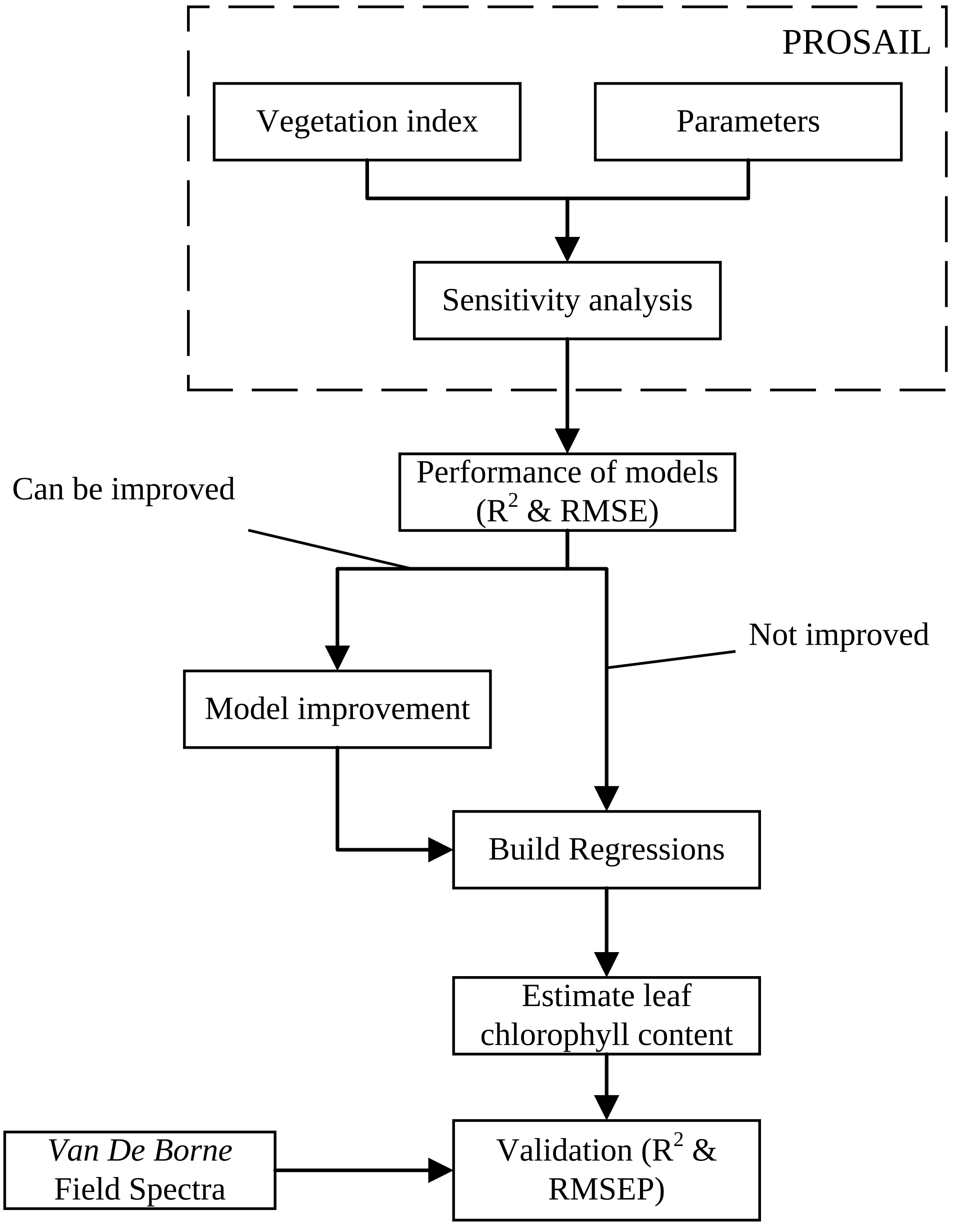

Figure 1: Flowchart of processes described for estimating leaf chlorophyll content using RTM and vegetation indices (Section 2)

2.2. Methods

The methods are subdivided into three parts. Firstly, a sensitivity analysis is performed using the different sensors (Section 2.1.4), the three vegetation indices (Section 2.1.5) and the suggested parameter variations (Section 2.1.3). Secondly, some of the outcomes of the initial sensitivity methods were found possible to improve. Two improvement methods were applied. After the improvements three models based on the different vegetation indices were created. Lastly, these three models were validated using the VDB spectra and known leaf chlorophyll contents (Section 2.1.1).

2.2.1. Sensitivity analysis

The PROSAIL model parameters and the vegetation indices (Table 2) were tested with a sensitivity analysis. The parameters (Table 1) were all loaded into ARTMO, which created 2160 PROSAIL simulations with a forward simulation. These simulations were loaded into ARTMO's 'spectral indices' package and the modelled parameter (leaf chlorophyll) was selected. This was followed by the selection of a vegetation index. ARTMO then computed how well the selected index performed. ARTMO presented a list of band combinations with several measures of error. This list was computed with 50% of the added data, where the selection of spectra was performed full-randomly. A part of this list is shown in Table 3 as an example.

Table 3: Example of results taken from ARTMO

Assessment table: ndvi

Class: Full_image | Variable: Cab | Type results: Calibration | Statistics: NRMSE | Top: 10 | ☐ No negative | OK

	Retri...	Graphics	SI	Fitting type	bands	spect_...	param_n...	model_tr...	user_train	MAE	RMSE	RRMSE	NRMSE
1	☐	☐	NDVI	linear	1375.0 705.0;	0	0	50	0	6.1212	7.4682	19.6982	9.9576
2	☐	☐	NDVI	linear	705.0 1375.0;	0	0	50	0	6.1212	7.4682	19.6982	9.9576
3	☐	☐	NDVI	linear	1610.0 705.0;	0	0	50	0	6.3421	8.0087	21.1237	10.6782
4	☐	☐	NDVI	linear	705.0 1610.0;	0	0	50	0	6.3421	8.0087	21.1237	10.6782
5	☐	☐	NDVI	linear	560.0 490.0;	0	0	50	0	6.4354	8.4172	22.2013	11.2230
6	☐	☐	NDVI	linear	490.0 560.0;	0	0	50	0	6.4354	8.4172	22.2013	11.2230
7	☐	☐	NDVI	linear	945.0 740.0;	0	0	50	0	5.9252	8.4699	22.3403	11.2932
8	☐	☐	NDVI	linear	740.0 945.0;	0	0	50	0	5.9252	8.4699	22.3403	11.2932
9	☐	☐	NDVI	linear	2190.0 560.0;	0	0	50	0	6.4650	8.6532	22.8238	11.5376
10	☐	☐	NDVI	linear	560.0 2190.0;	0	0	50	0	6.4650	8.6532	22.8238	11.5376

In this case the list is sorted by the Normalized Root Mean Square Error (NRMSE), so the sample on top has the best predictive power based on NRMSE. Within the list the band combination which most closely resembles the band combination of the selected vegetation index was selected manually. From the selection the user was able to collect data where a vegetation index was plotted against the selected parameter, leaf chlorophyll in this case. ARTMO was capable of giving results for any band combination provided. Another sensitivity analysis that was performed included several band selections of the sensors Sentinel-2 and VENμS. Because the bandwidth of these satellites are not equal this could cause issues for application purposes. Therefore, for instance for TCARI/OSAVI in Table 2 the band configuration might change within the index. The band combinations were obtained from either: Sentinel-2, VENμS or CropScan. The choice of band combinations is shown in Table 4.

Table 4: Selected spectral bands for the different sensors per vegetation index

	NDVI		**CVI**			**TCARI/OSAVI**			
	R_{RED} (nm)	R_{NIR} (nm)	R_{GREEN} (nm)	R_{RED} (nm)	R_{NIR} (nm)	R_{550} (nm)	R_{670} (nm)	R_{700} (nm)	R_{800} (nm)
SENTINEL-2	665	842	560	665	842	560	665	705	783
VENμS	620	865	555	667	865	555	667	702	782
CROPSCAN	670	870	550	670	870	550	670	700	780

All sensors had a minor difference with the wavelengths required in TCARI/OSAVI. These spectral bands were chosen for being in close proximity of the requirements. Although VENμS had a spectral band at 667nm, which was closer to 665nm, a choice was made to use the spectral band at 620nm. This was to test the sensitivity of the models based on NDVI with slightly different spectral bands in the same spectral region. The estimations of leaf chlorophyll were based on these spectral bands, so when validating between CropScan and one of the sensors there would be a minor systematic error between the estimated leaf chlorophyll based on the satellite sensor results and the measured leaf chlorophyll based on CropScan spectra.

When the proper band combination for the selected vegetation index was selected, the data was exported to R-Studio. Here, three regression fits were performed (linear, exponential, logarithmic). From these fits the Root Mean Squared Error (RMSE) and R^2 were calculated, using Equation 1 and Equation 2.

Equation 1: Root Mean Squared Error (of Prediction)

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

where, N = number of samples, y_i = observed value and $\hat{y}_i$ = predicted value

Equation 2: Coefficient of determination

$$R^2 \equiv 1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i (y_i - \bar{y})^2},$$

where y_i = observed value, $\hat{y}_i$ = predicted value and $\bar{y}$ = mean of observed data

The best regression fit was obtained from the fit with lowest RMSE, giving the most accurate result. The example in Table 3 showed a table sorted on NRMSE, but the RMSE was calculated outside of ARTMO. NRMSE is used to estimate the error between models using different scales, which was not the case for this study and thus the RMSE would suffice. An analysis with R^2 was done to see if the model made a precise regression. RMSE was also used in the validation stage, but here it was referred to as Root Mean Squared Error of Prediction (RMSEP). To specify what is considered sufficient for both estimators of error a minimum R^2 of 0.60 and minimum RMSEP of 50% of the observed mean are necessary.

2.2.2. Model improvement

The sensitivity analysis showed that some models could be improved. Two improvements were devised specifically for the outcomes of the sensitivity analysis. The first was Best Band Combination (BBC), which used the computational power of ARTMO. The second was Constraint, which cut the broad variation of parameters loaded into PROSAIL to resemble a more detailed and realistic situation of a given type of canopy (crop).

2.2.2.1. Best Band Combination

The Best Band Combination was obtained directly from ARTMO. Initially ARTMO calculated the best result for the applied fit. In Table 3 it can be seen that the best result for a linear fit for NDVI was obtained when spectral bands 705nm and 1375nm (Sentinel-2) were used. This spectral band combination was obtained by giving ARTMO the freedom to choose from all spectral bands the sensor contained. This method could give better results than the most commonly used bands for a given index. However, this method will not work well for an index that has some physical basis, like the TCARI/OSAVI. TCARI/OSAVI required pre-determined spectral bands at a certain wavelength, because it was developed as a vegetation index that takes the ratio between a crop chlorophyll estimator (TCARI) and a LAI estimator (OSAVI) (Haboudane et al., 2002). If the spectral bands would be chosen freely from all present spectral bands of a sensor, this index would be used out of context, making interpretation very difficult. However, letting the band combination free is sometimes done for a simple ratio vegetation index such as NDVI. The index that resulted was referred to as a pseudo-'index'. Interpretation of such combination could provide interesting results.

2.2.2.2. Constraint

The constraint improvement reduced a large range of a parameter into a more limited variation depending on what could be expected from the real situation. The constraint applied to the model in this study was a reduction in variation in the LAD parameter. The initial variation used was rather extreme concerning potato plants. Therefore, the range of LAD of 0˚ to 90˚ was adjusted to a more likely situation of 0˚ to 45˚. Because this parameter was of such interest the number of steps was also increased to four. The implemented LAD parameter in PROSAIL for the constrain improvement was 0˚, 15˚, 30˚ and 45˚. It followed that the number of forward simulations increased from 2160 to 2880 simulations. Such constrains could be applied to any of the parameters, however, this would make the model more specific to a certain vegetation, instead of giving a more generalized model.

2.2.3. Validation

Validation was done using the VDB data, as described in Section 2.1.1. For every year a separate dataset was created using the measured leaf chlorophyll and the CropScan spectra. These datasets were loaded into ARTMO. Again, using the 'spectral indices toolbox' the spectra were used to calculate the vegetation indices' values. These results were exported to R Studio where they were compared to the results from the sensitivity analysis. Comparison was done by plotting the validation results with the sensitivity analysis results and check whether the points were on the regression curve. The model based on sensitivity analysis results was transferred in a simple way onto the VDB spectra. The scatterplots that were created referred to a model transfer in their title. It was acknowledged that this was not a 'true' transfer as described in Fearn (2001). To test this, the vegetation index values of the validation were filled in the regression curves of the sensitivity analysis procedure. The estimations were then plotted against the measured values of the VDB spectra. However, for the Best Band Combination (Section 2.2.2.1) the model was built using the Sentinel-2 bands, which do not correspond at higher wavelengths with the CropScan sensor (Table 9 & Table 10). Therefore the model was validated using two band combinations. To simulate 705nm the wavelengths 700nm and 710nm were used and to simulate 1375nm the wavelengths 1050nm and 1650nm were used. Both combinations were investigated and plotted. No interpolation was performed. The R^2 (Equation 2) and RMSEP (Equation 1) were used to quantify the error.

3. Results

The results are structured as depicted in Section 2.1.6. Firstly, the results of the sensitivity analysis and model improvements are shown and sorted by vegetation index. Secondly, the models are validated on the Van De Borne spectral dataset.

3.1. Sensitivity Analysis

The sensitivity analyses were carried out by ARTMO using the parameters described in Section 2.1.3. Several improvements to the models were carried out according to the methods described in Section 2.2.2.

3.1.1. NDVI

The NDVI-based sensitivity results are shown in Figure 2.

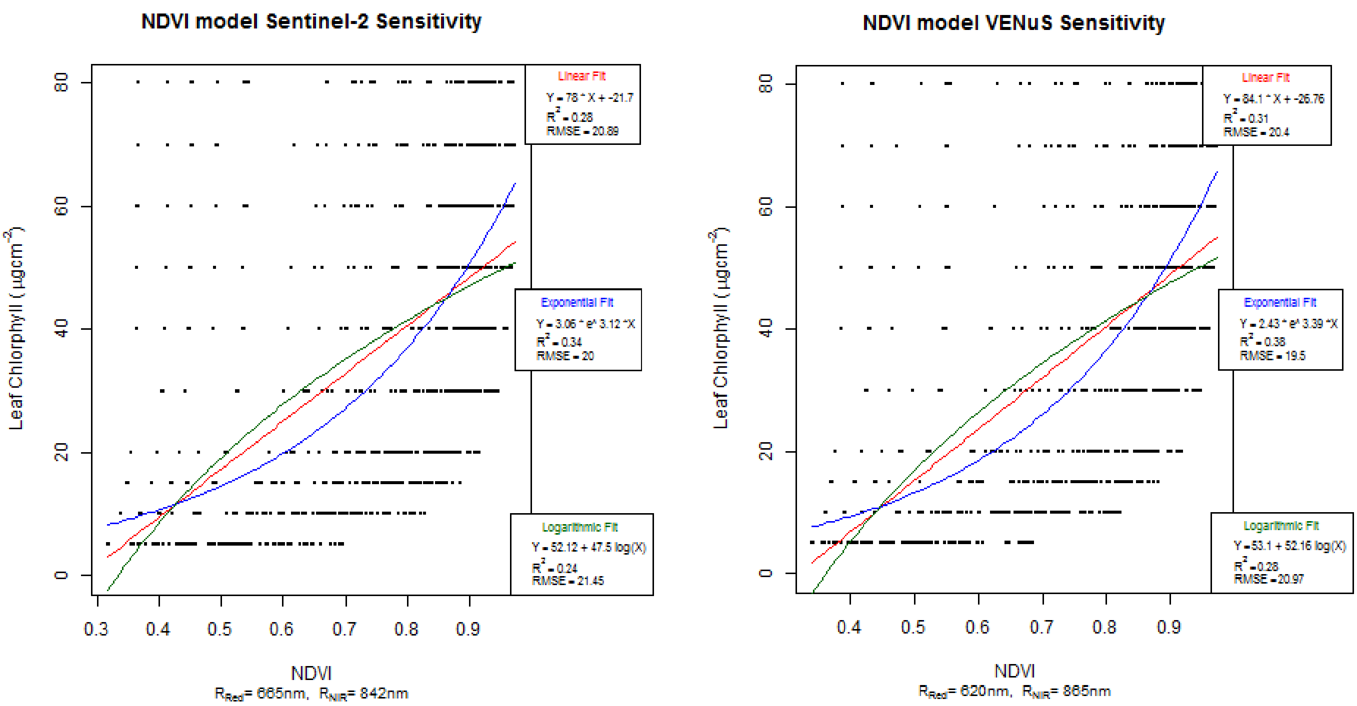

Figure 2: Simulated leaf chlorophyll concentration based on PROSAIL parameters using the NDVI index per sensor. Three different fitted functions are applied: linear, exponential and logarithmic.

A small difference in wavelengths can be recognized, because the VENµS sensor has an extra band in R_{Red} (620nm) and the Sentinel-2 band in R_{NIR} (842nm) is better centred in the NIR section of the spectrum than 865nm. These models are overall very sensitive to varying parameters, excluding leaf chlorophyll in the higher leaf chlorophyll ranges. The NDVI values are very spread for every leaf chlorophyll interval (0.3-0.7 at 5 µgcm^{-2} and 0.3-1.0 at 80 µgcm^{-2}). Coefficients of determination are very low for all fits with a best fit of R^2 = 0.38 for an exponential fit for the VENµS sensor. RMSE values are 20+ µgcm^{-2} for all fits, which is very high compared to the leaf chlorophyll range (5 – 80 µgcm^{-2}). Predictions with this model are expected to be very poor. The models based on the VENµS sensor perform better than the Sentinel-2 based models with about RMSE values of about 2 µgcm^{-2} lower and much better R^2 values. The best fit for the NDVI Sentinel-2 based model and the NDVI VENµS based model is an exponential fit.

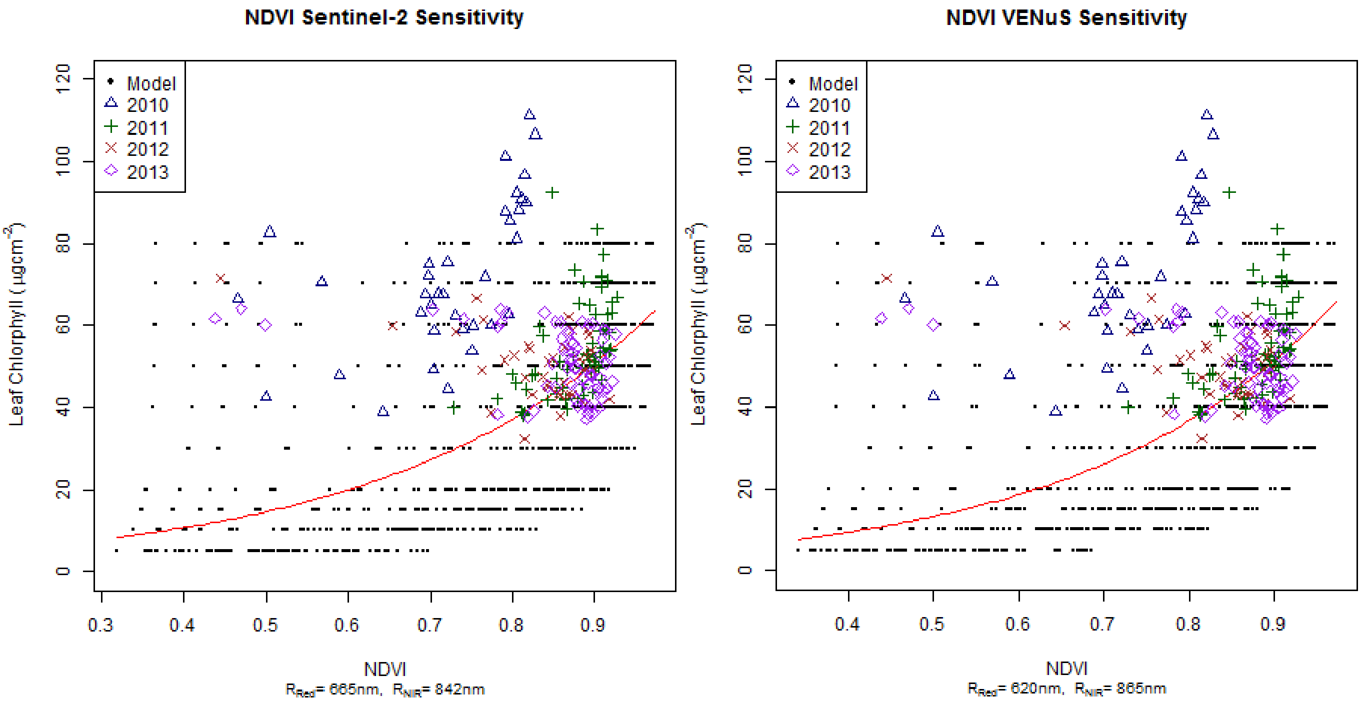

Figure 3: Simulated leaf chlorophyll concentration based on the PROSAIL parameters using the NDVI per sensor, with the VDB spectra for all four sampled years. An exponential fit is applied.

Figure 3 shows the outcomes of the VDB spectra when overlaid with PROSAIL. Important to note here is that the band configuration of the VDB spectra is slightly different as described in Section 2.2.1. The leaf chlorophyll of the VDB plants is mostly in the range of 40 – 70 µgcm^{-2}. The years 2011, 2012 and 2013 are very clustered within this range, with only a few outliers at lower NDVI values. The year 2010 has a more scattered pattern. Many 2010 samples exceeded 80 µgcm^{-2} and the samples have a lower NDVI than the samples of the other years.

Except for 2010 most points appear to fall within the sensitivity range of the upper leaf chlorophyll concentrations (40 – 80 µgcm^{-2}).

To improve the outcome of the NDVI sensitivity analysis a pseudo-NDVI is tested, as described in Section 2.2.2.1. The bands 705nm and 1375nm for Sentinel-2 and bands 620nm and 910nm for VENµS were chosen using ARTMO to decide which bands are the best combination for this analysis. These results are shown in Figure 4.

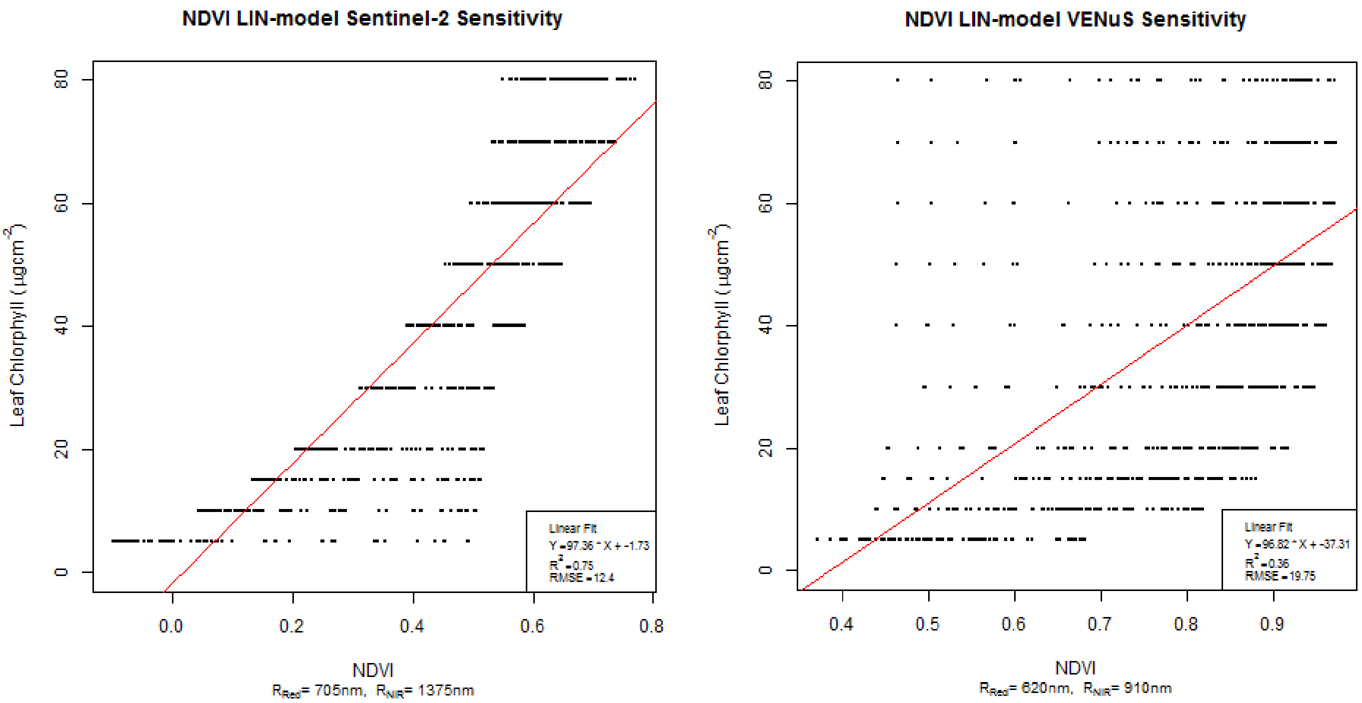

Figure 4: Simulated leaf chlorophyll concentration after Best Band combination based on PROSAIL parameters using the NDVI index per sensor. A linear fit is applied.

There is a big difference between both sensors in this result. The main cause of this is likely the importance of the R_{NIR} band (1375nm) in the Sentinel-2 sensor, which lacks in the VENµS sensor. The RMSE and R^2 of the sensitivity analysis based on the NDVI in Sentinel-2 have improved in comparison to the traditional NDVI bands (RMSE = 20.00 µgcm^{-2} (exponential fit) to RMSE = 12.40 µgcm^{-2} (linear fit) and R^2 = 0.34 (exponential fit) to R^2 = 0.75 (linear fit)). The relationship between leaf chlorophyll and NDVI has changed into a linear relationship from an exponential relationship. Only a linear relationship is presented, because after the best band combination improvement the best fit was a linear fit. However, the VENµS results still show a more exponential relationship and its results resemble the results of the previous analysis.

Overall the model is rather sensitive to the parameters varied. There is still a high overall sensitivity to LAI and to lesser extent leaf chlorophyll. At higher concentrations of leaf chlorophyll the model becomes more insensitive to leaf chlorophyll.

The VDB results have been plotted with the improved NDVI based model outcomes. Two plots are depicted according to Section 2.2.2.1 (Figure 5). Important to note here is that the spectral bands are slightly different, as was described in Section 2.2.3.

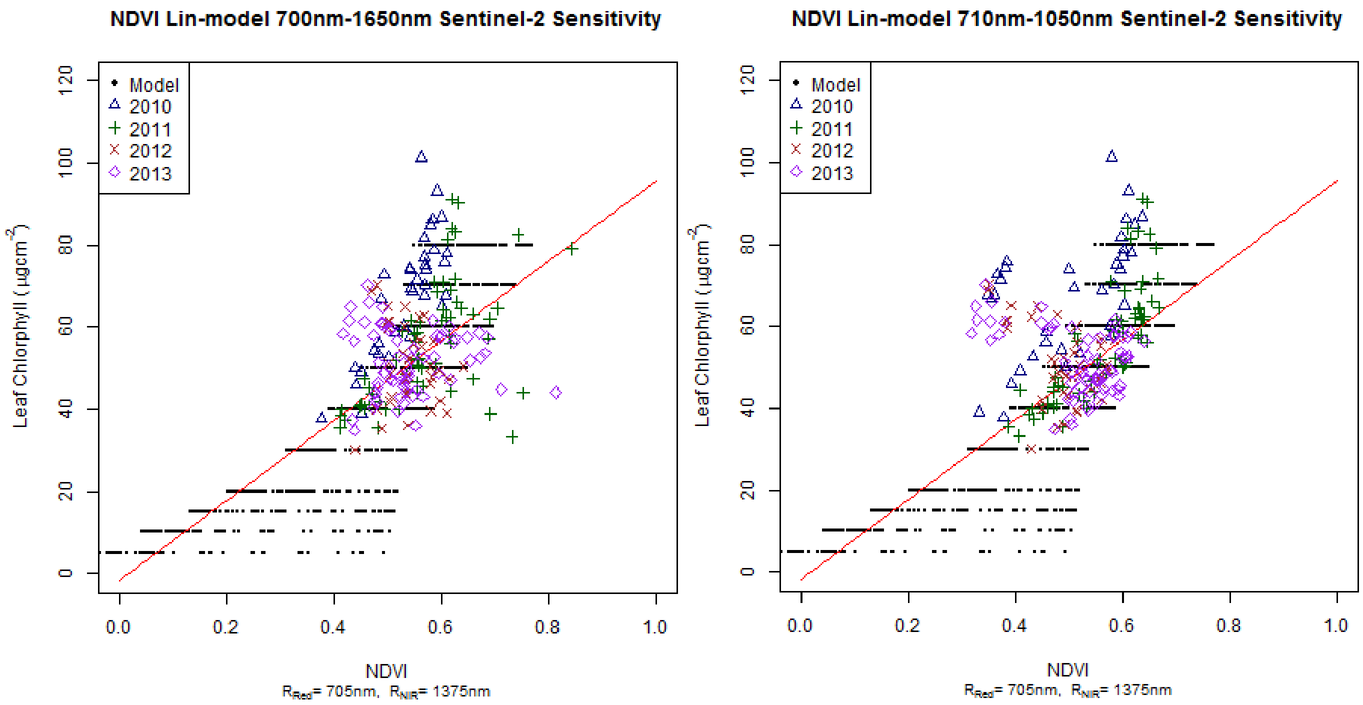

Figure 5: Simulated leaf chlorophyll concentration based on the PROSAIL parameters using the Best Band NDVI combinations, with the VDB spectra for all four sampled years. A linear fit is applied.

The NDVI based models do not perform well for this analysis. In both plots the points do not align with the fitted line. Between 40 µgcm^{-2} and 60 µgcm^{-2} the points of the years 2011 and 2013 seem to follow the fitted line. The NDVI based model with the VDB data using bands 710nm and 1050nm appear slightly more accurate in this region than the NDVI based model with VDB bands 700nm and 1650nm. However, spread is too large to suggest anything about accuracy. Overall, most points are included in the parameter ranges, but for all years there are plenty of outliers.

3.1.2. CVI

The following sensitivity models are based on the CVI. The results are based on the method presented in Section 2.2.1. The outcome of the sensitivity analysis on the CVI based models is shown in Figure 6.

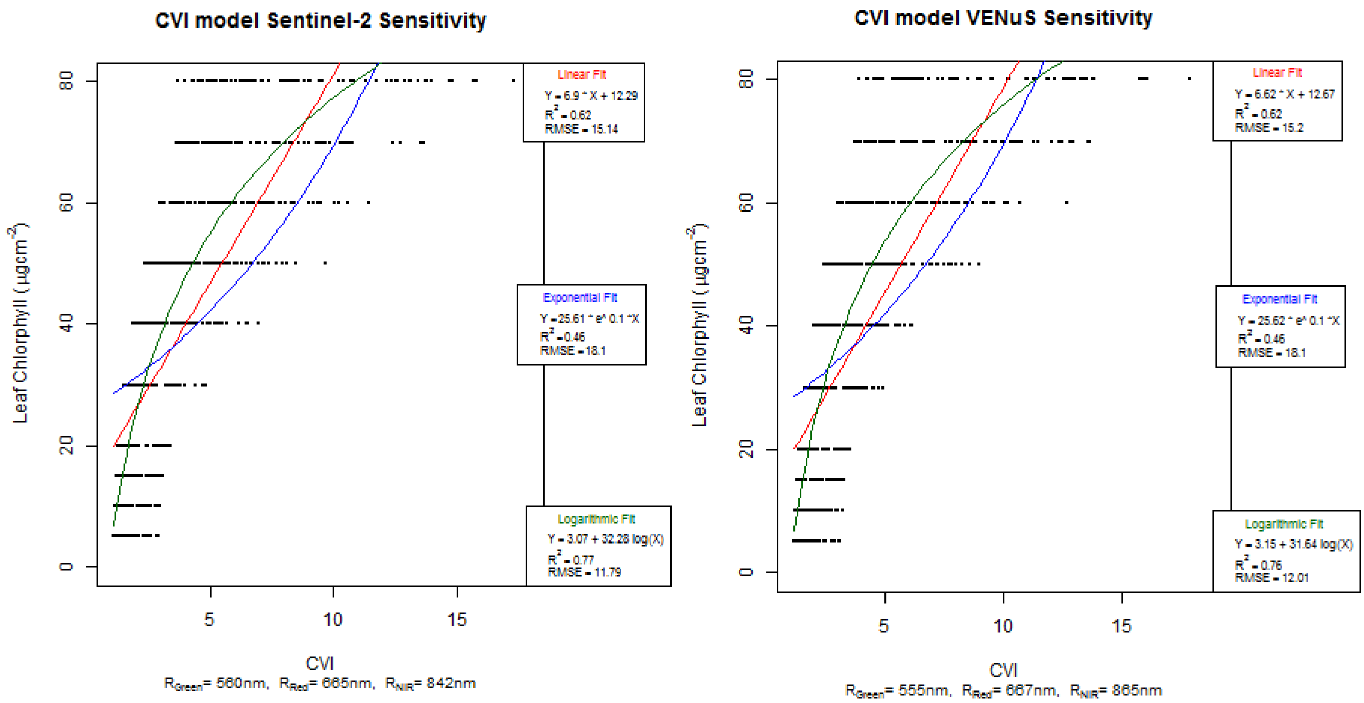

Figure 6: Simulated leaf chlorophyll concentration based on PROSAIL parameters using the CVI index per sensor. Three different fitted functions are applied: linear, exponential and logarithmic.

The models based on the CVI for both sensors performed much better than the NDVI models. The sensitivity of the model can be better assessed than the NDVI-models' sensitivity. The models for both sensors are insensitive for a change in parameters at low concentrations (< 40 µgcm^{-2}) of leaf chlorophyll. At higher concentrations sensitivity increases, because the spread of CVI at the leaf chlorophyll intervals increases. The best fit for both sensors is a logarithmic fit ($R^2_{Sentinel\text{-}2} = 0.77$ and $R^2_{VEN\mu S} = 0.76$). The performance of the models is not significantly different between sensors ($RMSE_{Sentinel\text{-}2} = 11.79$ µgcm^{-2} and $RMSE_{VEN\mu S} = 12.01$ µgcm^{-2}). A similar wavelength choice has been made for the NIR section of the spectrum as for the NDVI models (842nm instead of 865nm).

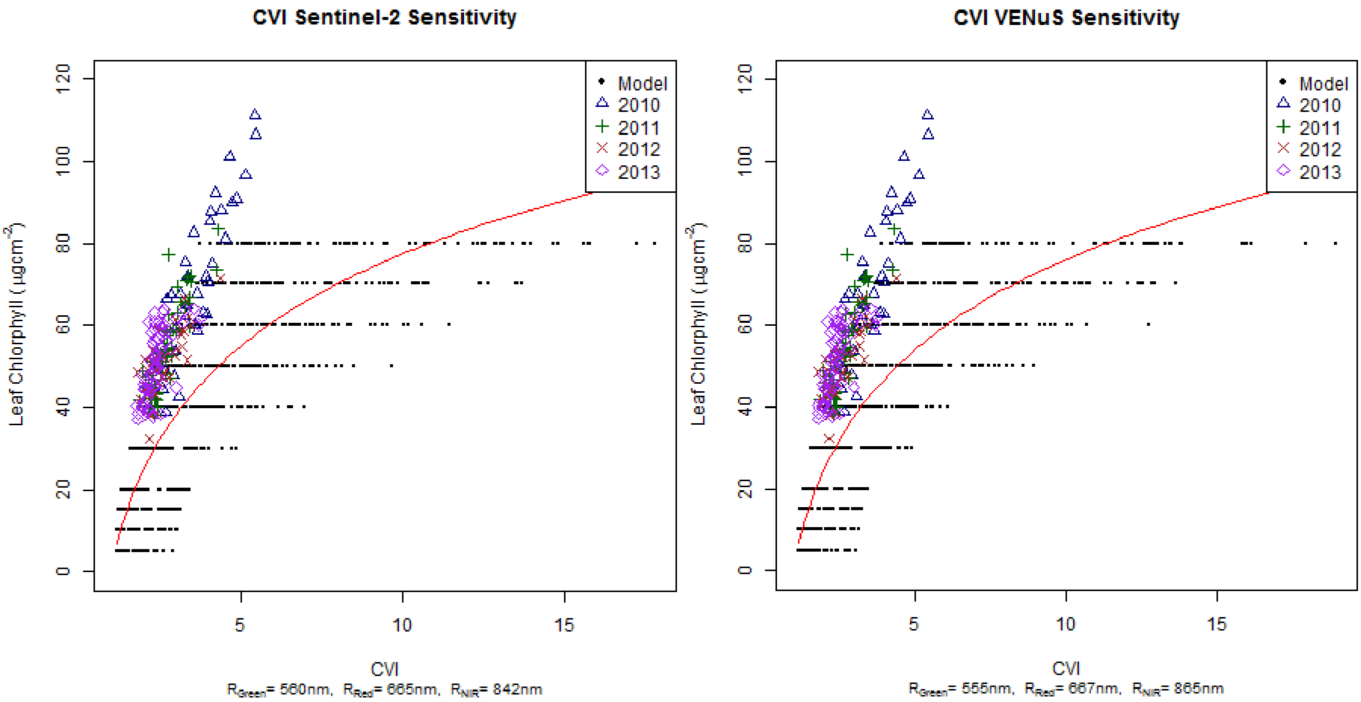

Figure 7: Simulated leaf chlorophyll concentration based on the PROSAIL parameters using the CVI per sensor, with the VDB spectra for all four sampled years. A logarithmic fit is applied.

In Figure 7 the VDB PROSAIL outcomes are plotted with the sensitivity results. Compared to the NDVI model the samples are spread less. A clear offset can be seen when comparing the modelled sensitivity with the VDB results. This could be caused by the large range of LAD. The trend of the VDB CVI values followed a linear fit instead of the modelled logarithmic fit. The CVI values of the VDB spectra are lower for the measured leaf chlorophyll than the model suggests. The CVI for the VDB spectra appears to have a more linear relationship with the leaf chlorophyll content instead of a logarithmic fit.

3.1.3. TCARI/OSAVI

The TCARI/OSAVI based models were plotted in Figure 8. TCARI/OSAVI requires a band with a wavelength of 800nm (Table 2). However, for this analysis bands $R_{Sentinel\text{-}2}$ = 783nm and $R_{VEN\mu S}$ = 782nm are used.

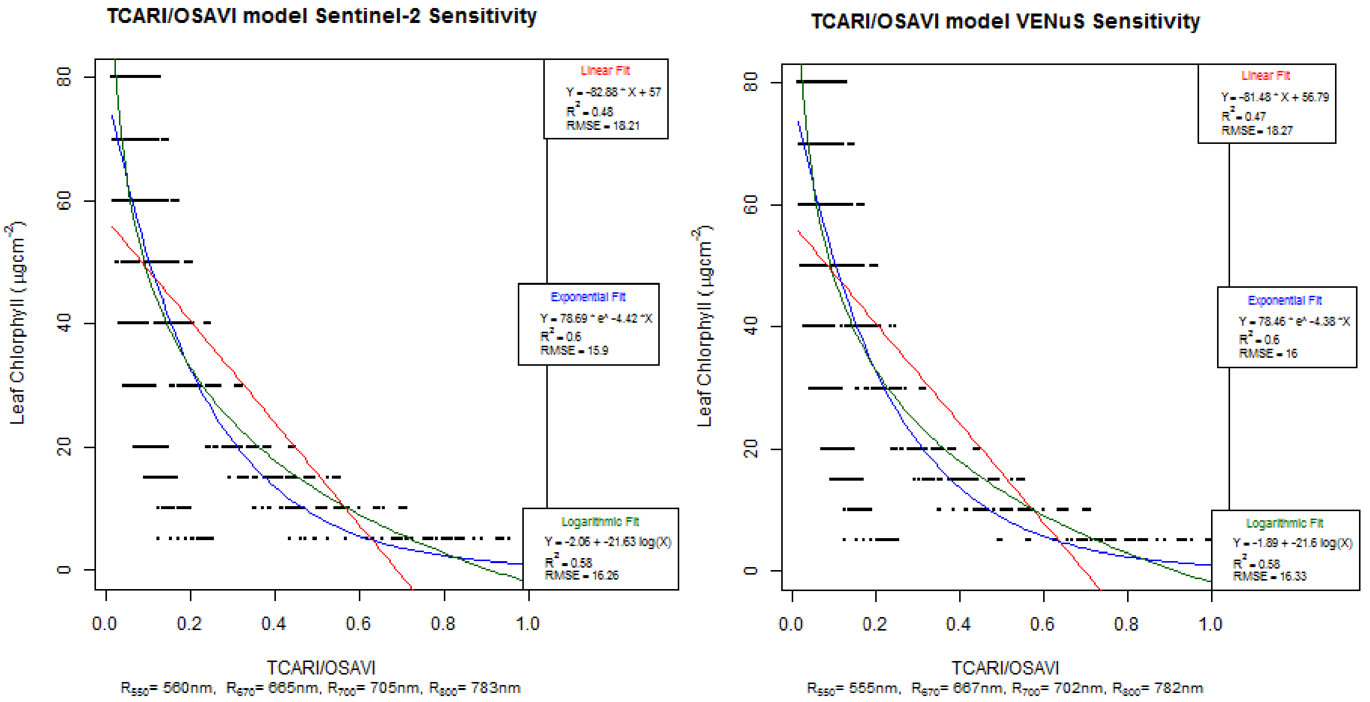

Figure 8: Simulated leaf chlorophyll concentration based on PROSAIL parameters using the TCARI/OSAVI index per sensor. Three different fitted functions are applied: linear, exponential and logarithmic.

The TCARI/OSAVI appears to be less sensitive to higher leaf chlorophyll concentrations opposed to the CVI. TCARI/OSAVI shows much more spread at lower leaf chlorophyll concentrations. However, this spread might be caused by one of the parameters. It can be seen that the spread is caused by a break between model results. Around 30 μgcm^{-2} a divergence of the results can be seen, whereas most of the results fall within the exponential fit with higher TCARI/OSAVI values (0.5-1.0 at 5 μgcm^{-2}), a part of the model results stay at a lower TCARI/OSAVI value (0.1-2.5 at 5 μgcm^{-2}). There is almost no difference in sensors ($R^2_{Sentinel\text{-}2} = R^2_{VEN\mu S}$ = 0.60, $RMSE_{Sentinel\text{-}2}$ = 15.90 μgcm^{-2} and $RMSE_{VEN\mu S}$ = 16.00 μgcm^{-2}).

To improve these results of this sensitivity analysis the parameter LAD was constrained according to Section 2.2.2.2. The result of this procedure are shown in Figure 9.

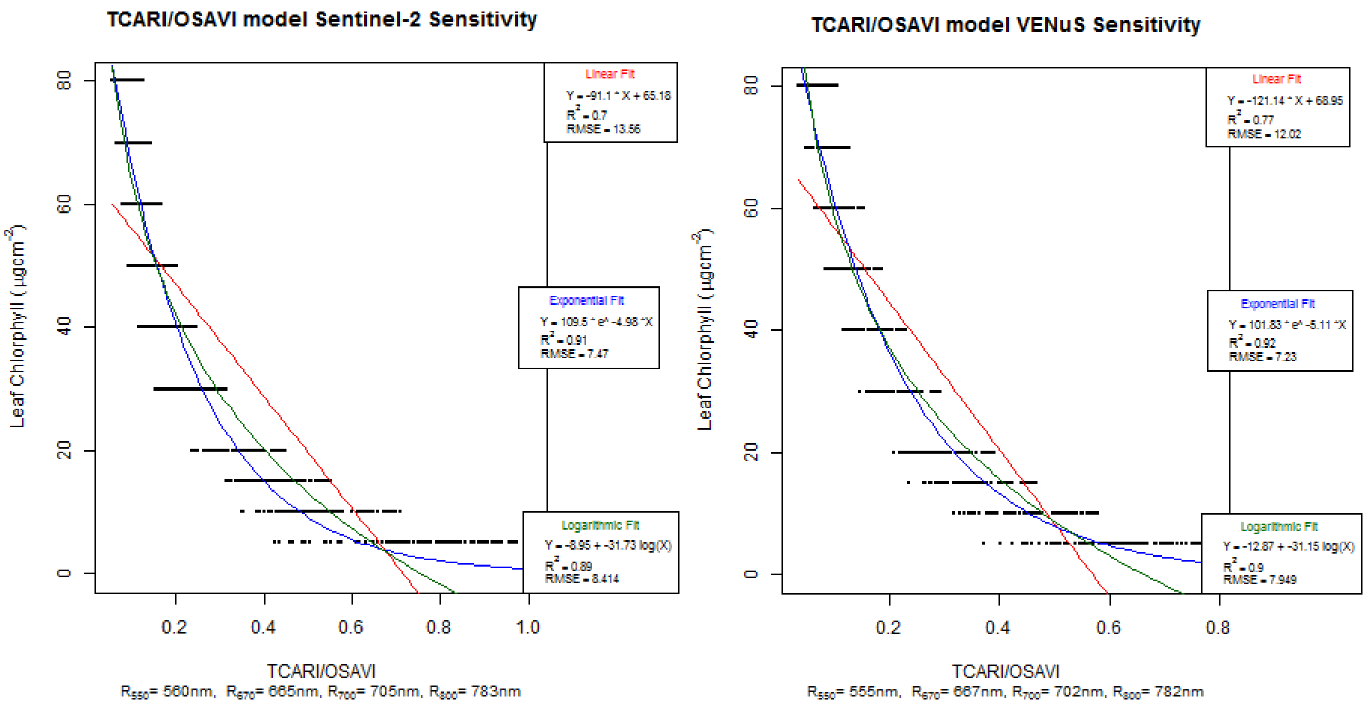

Figure 9: Simulated leaf chlorophyll concentration after constraint based on PROSAIL parameters using the TCARI/OSAVI per sensor. Three different fitted functions are applied: linear, exponential and logarithmic.

After constraining the range of LAD much better results were achieved. For the model based on the Sentinel-2 sensor it was found that the RMSE decreased from $RMSE_{unconstrained}$ = 15.90 µgcm^{-2} to $RMSE_{constrained}$ = 7.47 µgcm^{-2}. The R^2 increased from 0.60 to 0.91. The model's performance based on VENµS was similarly improved where RMSE decreased from 16.00 µgcm^{-2} to 7.23 µgcm^{-2} and R^2 increased from 0.60 to 0.92. The misfits in previous models were caused by the large range of LAD used to test sensitivity. At high leaf chlorophyll concentrations TCARI/OSAVI is quite insensitive to both LAI and leaf chlorophyll. It can be seen that the spread at these higher concentrations is small resembling insensitivity for LAI and the insensitivity in leaf chlorophyll can be assumed from the steepness of the fit. This steepness shows that the index value is not changing much, but the leaf chlorophyll is increasing in concentration.

In Figure 10 the modelled and constrained TCARI/OSAVI is plotted with the VDB results.

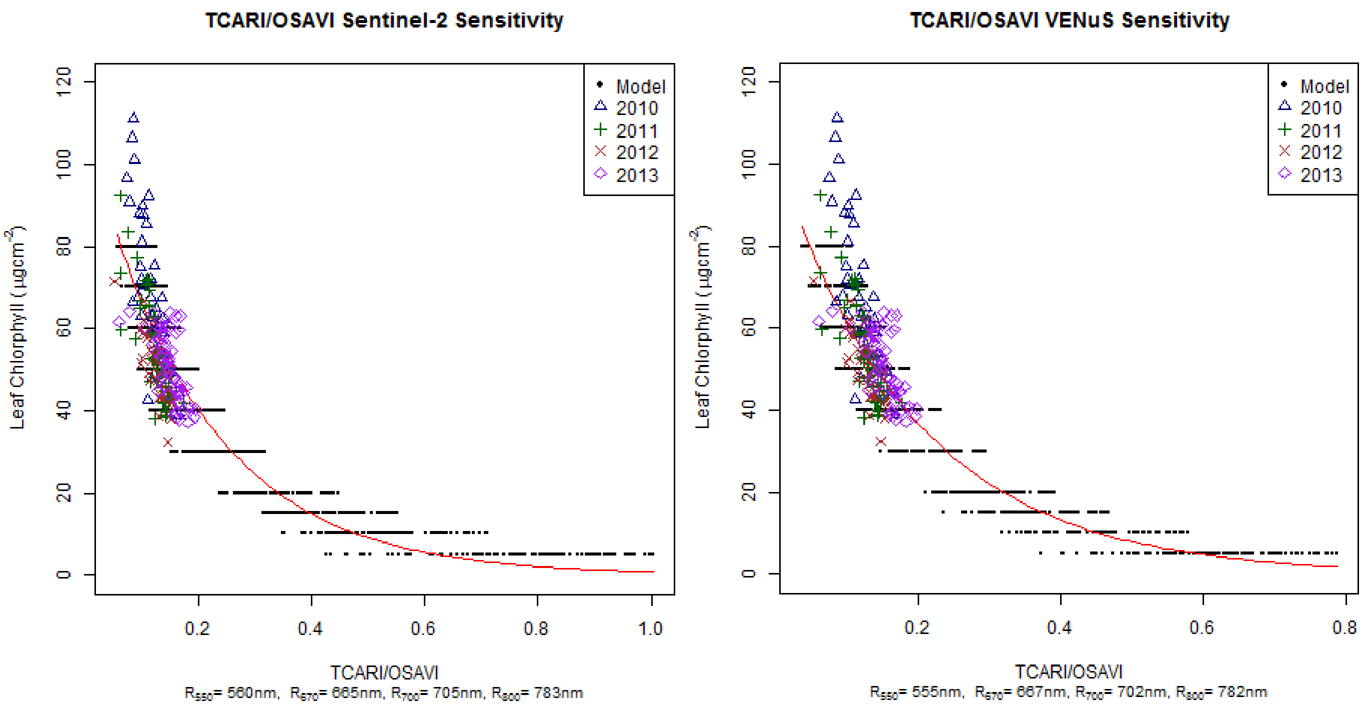

Figure 10: Simulated leaf chlorophyll concentration based on the constraint PROSAIL parameters using the TCARI/OSAVI per sensor, with the VDB spectra for all four sampled years. An exponential fit is applied.

The VDB points nearly all fall within the range of the model. Again, the large leaf chlorophyll concentrations of the year 2010 have not been accounted for. The point cloud of the VDB data follows the fit rather well. However, there is a difference between sensors. The Sentinel-2 based model appears to perform a bit better at higher leaf chlorophyll concentrations (70-80 µgcm^{-2}). The VDB points are closer to the fitted line than for the VENµS based model. On the other hand the VENµS based sensor seems to perform a little better at lower concentrations (40-50 µgcm^{-2}) than the Sentinel-2 based models, there are more points on the fitted line.

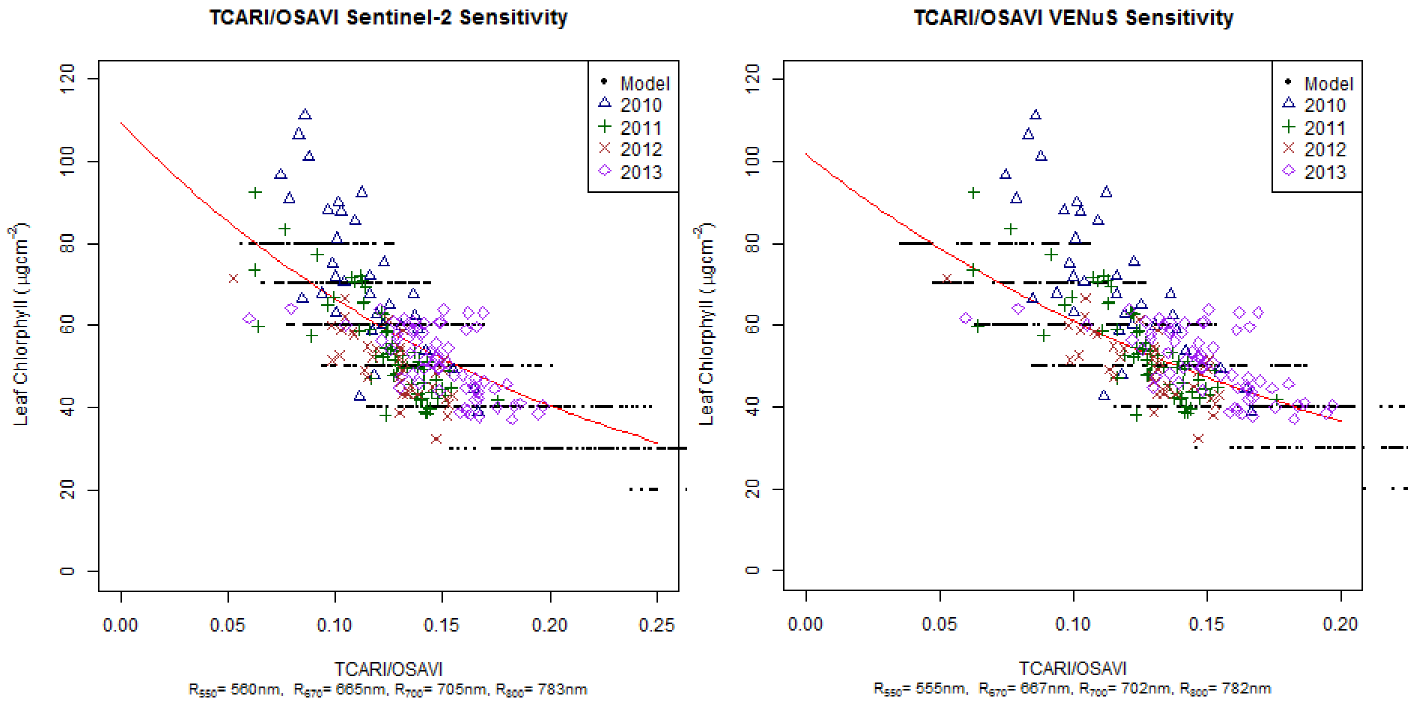

Figure 11: Simulated leaf chlorophyll concentration based on the constraint PROSAIL parameters using the TCARI/OSAVI per sensor, with the VDB spectra for all four sampled years on a smaller scale (0.0 - 0.25). An exponential fit is applied.

Figure 11 are two plots where the TCARI/OSAVI scale was reduced to 0 – 0.25 to investigate the regression in more detail. The year 2010 does not fit with the exponential regression curve as was already mentioned above. The year 2013 appears to fit less with the curve for the model based on the VENμS, because most of the points are clustered above the regression curve. The fit between the other two years (2011 and 2012) seems to be better, with less difference between sensors.

3.2. Modelled Leaf Chlorophyll estimations

The modelled regressions based on the results of the sensitivity analysis with PROSAIL were used to create estimations of leaf chlorophyll using the CropScan spectral measurements. These estimations were compared with the real leaf chlorophyll values found in the field.

3.2.1. NDVI

The following results are the outcomes of the modelled regression estimation according to Section 2.2.3. The leaf chlorophyll estimated by the NDVI based regressions are shown in Figure 12.

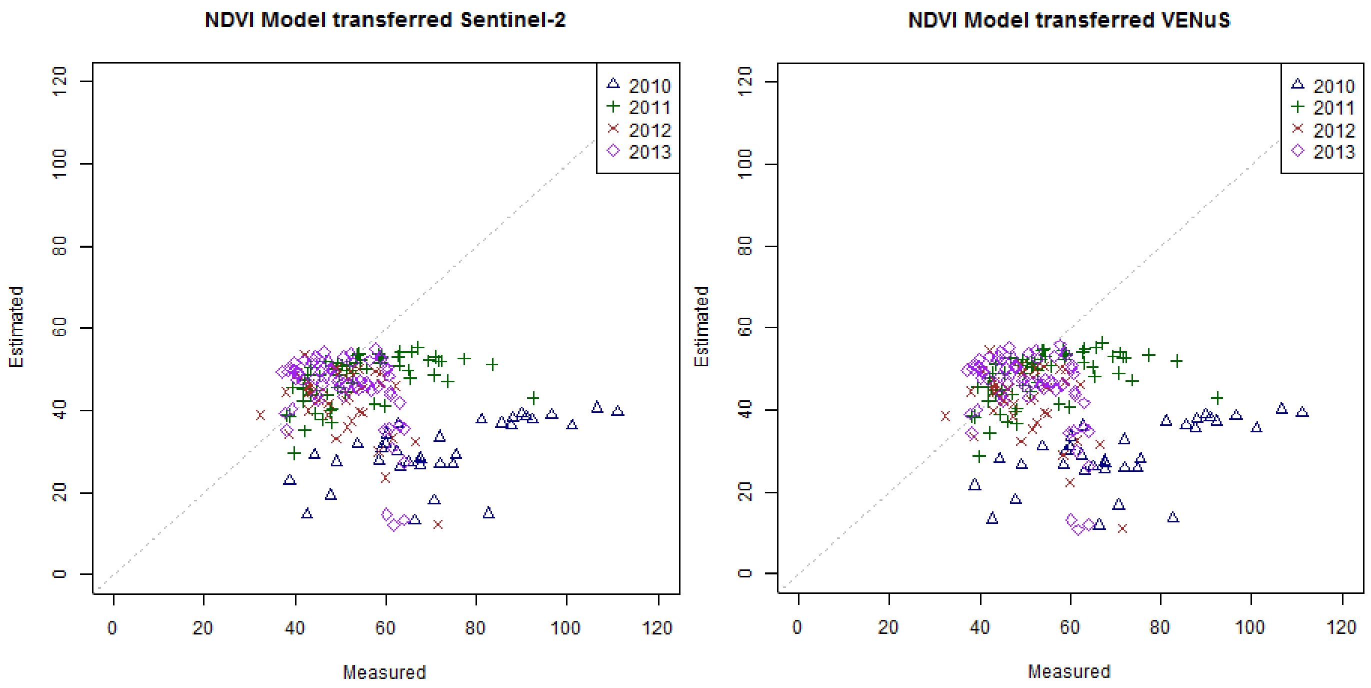

Figure 12: Plots of estimations of leaf chlorophyll (µgcm^{-2} for the four measurement years of the VDB fields) built with the NDVI based model for the two different sensors: Sentinel-2 and VENµS.

The performance of the regression built from the NDVI based models in the previous section, Section 3.1, is not so good. Considering the results in Figure 2 this was expected. Especially for the years 2010 and 2011 most estimations are plotted in a horizontal pattern, not following the one to one line. This means that the model estimates the same leaf chlorophyll concentration at different index values. Results for 2013 are a little better, however, around 60 µgcm^{-2} a lot higher concentrations are measured than estimated. Neither does it seem to estimate values higher than 60 µgcm^{-2}. To further illustrate the performance of the regression the R^2 and RMSEP are shown in Table 5:.

Table 5: Comparison of measures of error: R^2 and RMSEP of two different sensors: Sentinel-2 and VENμS, based on the leaf chlorophyll estimations created by the NDVI based model.

	SENTINEL-2		**VENUS**	
	R^2	RMSEP	R^2	RMSEP
2010	0.381	44.32	0.389	45.10
2011	0.243	12.52	0.244	12.33
2012	0.179	16.47	0.175	16.88
2013	0.189	15.82	0.189	16.20

The year 2010 performs the least of all years. The R^2 is the highest, but Figure 12 showed a very horizontal pattern for this year, resulting in a better R^2 than for the other years. RMSEP is high for all models considering the range of estimations are between 20 and 60 μgcm^{-2}. Improvements to this method were made and the results of these were shown in Figure 13.

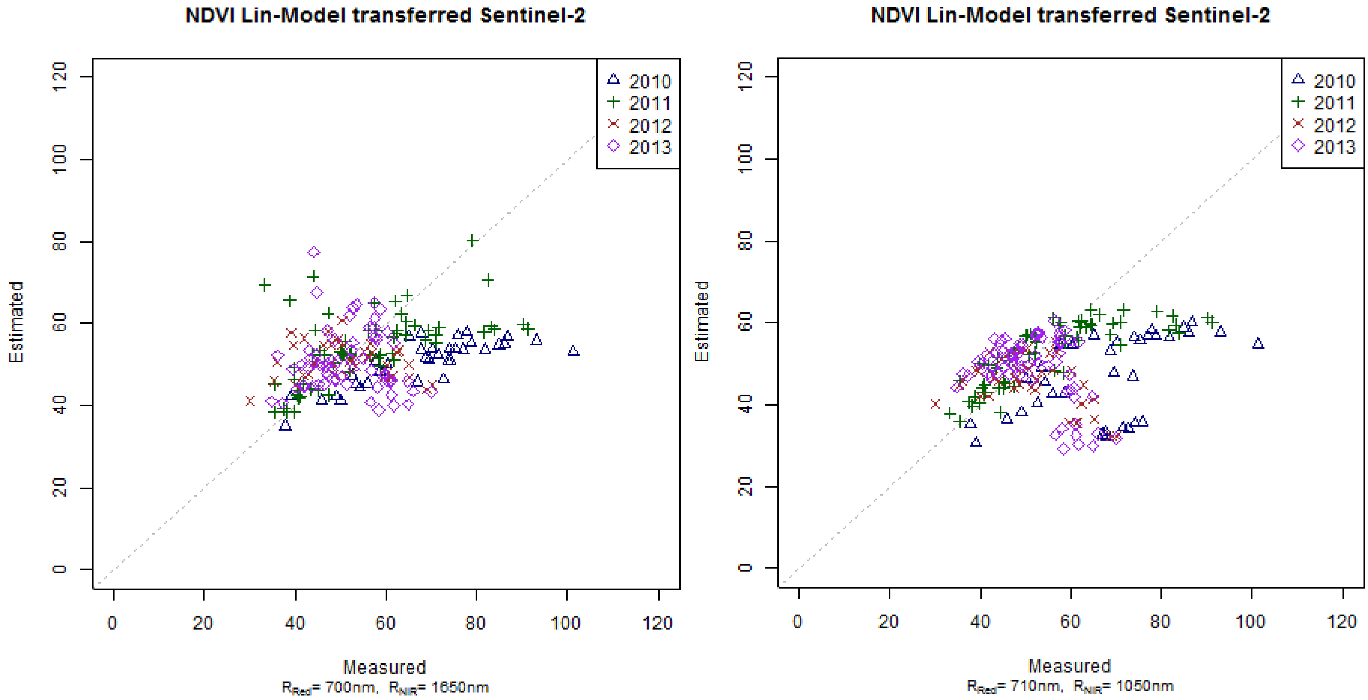

Figure 13: Plots of estimations of leaf chlorophyll (μgcm^{-2}) for the four measurement years of the VDB fields built with the 'best band' NDVI based model for Sentinel-2.

The outcomes of the improved NDVI based model regression are slightly better than the regression results of the regular NDVI based model shown previously. The points are slightly better positioned around the one to one line and the spread of the points is smaller. There is also less of a horizontal pattern to be observed. Especially the VDB data of 2011 in the NDVI based model regression using bands 710nm and 1050nm appear to perform much better, with only a visible saturation around 60 µgcm^{-2}. However, this saturation is less apparent in the NDVI based model regression using bands 700nm and 1650nm, where some estimations are more than 60 µgcm^{-2}. The performance is again further illustrated by Table 6.

Table 6: Comparison of measures of error: R^2 and RMSEP of two different band configurations: 700-1650nm and 710nm-1050nm, based on the leaf chlorophyll estimations created by the 'best band' NDVI based model.

	700NM - 1650NM		**710NM - 1050NM**	
	R^2	RMSEP	R^2	RMSEP
2010	0.653	20.52	0.306	24.39
2011	0.312	12.24	0.633	10.12
2012	0.008	10.94	0.178	14.54
2013	0.001	11.26	0.153	13.65

Again, the NDVI based model regression (700nm – 1650nm) has a good R^2 for the year 2010. In Figure 13 (700nm – 1650nm) it can be seen that the estimations for the year 2010 are scattered linearly, resulting in a good R^2. However, this linear cluster of points for 2010 does not estimate leaf chlorophyll content well, because it is scattered far from the one-to-one line, resulting in a high RMSEP. The RMSEP values are overall rather high, therefore these models have a poor performance. The VDB data of 2011 are predicted quite well using bands 710nm and 1050nm, with the lowest RMSEP of 10.12 µgcm^{-2}, a R^2 of 0.63 and most points are positioned on the one to one line. However, for the two consecutive years R^2 is very low and there is no correlation between estimated and measured values.

3.2.2. CVI

The CVI based model regressions were plotted in Figure 14. The bands used were similar to the previous band choice in the sensitivity analysis of Section 3.1.2.

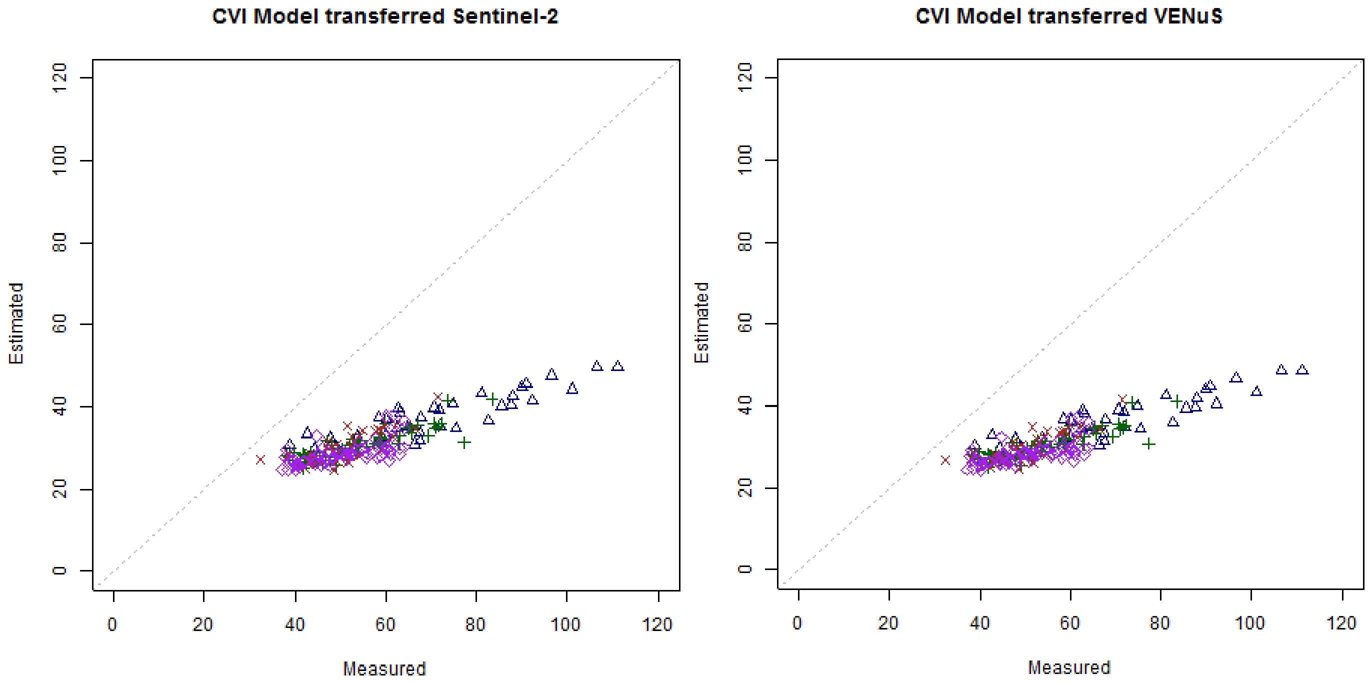

Figure 14: Plots of estimations of leaf chlorophyll (µgcm^{-2}) for the four measurement years of the VDB fields built with the CVI based model for the two different sensors: Sentinel-2 and VENµS.

The estimations for both sensors follow a horizontal pattern, showing very bad predictive performance. All VDB data follow this pattern. The data points are all positioned underneath the one to one line meaning that the model's regression estimations are underestimated. These horizontal patterns cause the R^2 to be rather good, the estimations are precise, but not accurate (Table 7). The RMSEP values of these regressions were worse than the RMSEP values of the regression of the NDVI based models (Table 6).

Table 7: Comparison of measures of error: R^2 and RMSEP of two different sensors: Sentinel-2 and VENµS, based on the leaf chlorophyll estimations created by the CVI based model.

	SENTINEL-2		VENUS	
	R^2	RMSEP	R^2	RMSEP
2010	0.780	36.58	0.780	37.26
2011	0.740	24.61	0.740	24.99
2012	0.620	21.32	0.620	21.67
2013	0.433	23.22	0.433	23.51

3.2.3. TCARI/OSAVI

The TCARI/OSAVI based models were plotted in Figure 15. However, for this analysis only the constrained TCARI/OSAVI model was used, because of its much more improved performance.

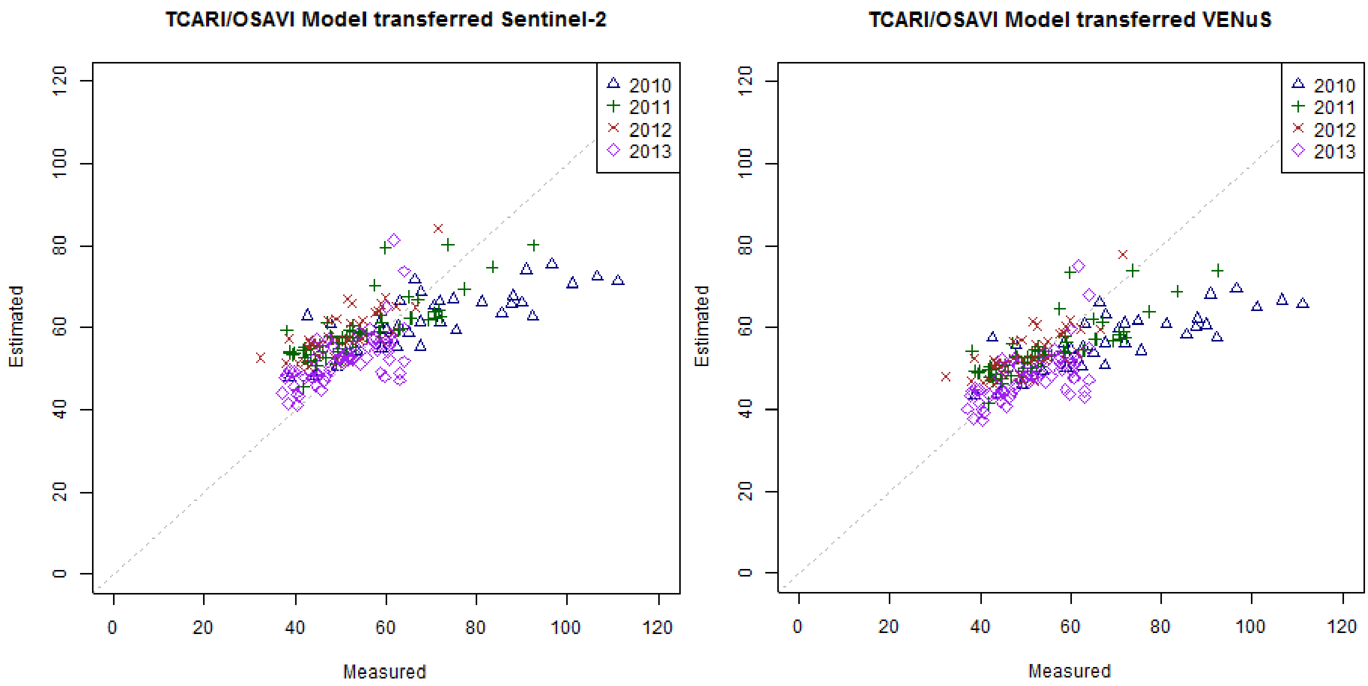

Figure 15: Plots of estimations of leaf chlorophyll (μgcm^{-2}) for the four measurement years of the VDB fields built with the constraint TCARI/OSAVI based model for the two different sensors: Sentinel-2 and VENμS.

TCARI/OSAVI appears to be performing the best out of all the indices used. The VDB data follow a pattern along the one to one line. The VDB data from the years 2011 and 2013 follow this one to one line very well. However, the VDB data from 2012 were slightly overestimated. The VDB data of 2010 were underestimated at higher concentrations of leaf chlorophyll. There is a minor difference between sensors, the results in the model regression based on Sentinel-2 seem to be more overestimated than the results in the model regression based on VENμS. This can also be spotted in the model's performance in Table 8. The R^2 values are quite good except for the VDB data of 2013. For the VDB data of the years 2011-2013 RMSEP for the VENμS based model regression is lower than the Sentinel-2 based model regression. At a minimum RMSEP of 6.40 μgcm^{-2} around the mean of (~) 60 μgcm^{-2} it could be said this model regression is quite good.

Table 8: Comparison of measures of error: R^2 and RMSEP of two different sensors: Sentinel-2 and VENµS, based on the leaf chlorophyll estimations created by the constrained TCARI/OSAVI based model.

	SENTINEL-2		**VENµS**	
	R^2	RMSEP	R^2	RMSEP
2010	0.586	16.42	0.586	19.90
2011	0.650	8.87	0.650	7.66
2012	0.564	9.94	0.563	6.40
2013	0.377	6.80	0.376	7.32

4. Discussion

4.1. NDVI

The NDVI is a commonly used index in biomass and canopy estimations and its purpose in this research was to compare the wide use of this index with indices that are more specialised towards leaf property estimations. Therefore, the expectations of this index were low. The NDVI results gave an insight towards the effects of the spectral band definitions and different sensors. The results of the models based on the NDVI were improved with a Best Band Combination method, which opened an interesting idea towards estimating leaf chlorophyll by using a ratio index.

The NDVI was clearly outperformed by the other two indices (CVI and TCARI/OSAVI). The sensitivity analysis showed that the model based on NDVI was highly sensitivity to most PROSAIL parameters (Figure 2). The spread over the leaf chlorophyll intervals was very high. The sensitivity of leaf chlorophyll itself seems to decrease at higher simulated leaf chlorophyll contents. NDVI is known to be highly sensitive to low LAI values (< 3) and saturate at higher levels of LAI (Asrar, Fuchs, Kanemasu, & Hatfield, 1984). Because the LAI range went until 6 a large part of the spread could be attributed to this behaviour of NDVI at lower LAI values. Another cause of the spread could be caused by a rather extreme range of LAD. The range of LAD for the simulations was from planophile – spherical – erectophile. The effect of LAD was clearly observed in the TCARI/OSAVI sensitivity analysis (Figure 8 & Figure 9), however, it was less apparent in the NDVI sensitivity analysis after comparison. Due to this spread a proper regression model could not be created. As Table 5 presented the R^2 were all very low (< 0.40) for every fit tried (linear, exponential and logarithmic). The best fit for both sensors was an exponential fit ($RMSE_{Sentinel\text{-}2}$ = 20 µgcm^{-2} and $RMSE_{VEN\mu S}$ = 19.5 µgcm^{-2}), but the RMSE is too high considering a mean of the leaf chlorophyll range of 42.5 µgcm^{-2}. The NDVI based models were clearly not able to be used for predicting leaf chlorophyll.

There was a slight difference in the selected spectral band definitions (Table 4). VENµS possesses a band with a wavelength 620nm which gave better results in the RED than 667nm in the Visible spectral region and the Sentinel-2 bands had a slightly better focus around the Red-Edge. However, for the results it made no real difference, considering the already high spread due to the sensitivity to the PROSAIL parameters. A small improvement of the regressions can be observed for the VENµS based results compared to the Sentinel-2 results. However, nothing conclusive can be said about these results, due to the large errors in: sensitivity, low R^2 and large RMSE. The validation with the VDB spectra showed again the effect of the large spread on the predictive power of the NDVI based models (Figure 3). Except for the year 2010, the VDB spectra are positioned in a rather vertically oriented point cloud at a NDVI value of 0.9. Although the exponential regression fit does fit some points, it can be clearly observed that the point cloud does not follow the regression line. The sampled year 2010 showed some very high leaf chlorophyll contents which could not be explained by PROSAIL, because the maximum input value of the leaf chlorophyll parameter for the simulations was 80 μgcm^{-2}. The effect was likely caused by its treatment with increased nitrogen fertilization (Clevers & Kooistra, 2014) and is therefore out of scope of this research.

To improve the model a Best Band Combination was tried (Section 2.2.2.1). The analysis based on the VENµS spectral bands was only slightly improved by this method. However, the sensitivity analysis based on Sentinel-2 was greatly improved, RMSE decreased from 20 μgcm^{-2} to 12.4 μgcm^{-2}, and the best fit became linear. The wavelengths for this improvement were 705nm and 1375nm. This resulted in a different ratio index as defined in Equation 3.

Equation 3: Formulation of an undefined ratio index, using a SWIR and a Red-Edge band

$$Ratio\ index = \frac{\lambda_{1375} - \lambda_{705}}{\lambda_{1375} + \lambda_{705}}$$

The wavelength of 705nm is positioned just at the start of the Red-Edge region and the wavelength 1375 is positioned between NIR and MIR, and is used for cirrus detection. So, leaf chlorophyll seems to be better predicted by a normalized difference between a water sensitive band and a Red-Edge band. Defined as such, it is related to the Normalized Difference Water Index (NDWI) (Gao, 1996). In the Red-Edge region the reflectance of leaf chlorophyll rapidly changes from low reflectance to high. In the water sensitive reflective signal in vegetation a rapid decline from high reflectance to low reflectance can be observed. The Red-Edge band is known to be very sensitive to leaf chlorophyll (Kooistra & Clevers, 2016). The 1375nm band is very close to 1400nm, where the atmosphere does not transmit any radiation, hence the use in cirrus detection. Gao (Gao, 1996) used the spectral bands 860nm (NIR) and 1240nm for the NDWI. The major difference between these two related indices is the use of Red-Edge spectral band (705nm) instead of a spectral band in NIR (860nm).

When validating the VDB spectra with the outcome of the improved NDVI based model the results are much better. However, due to the CropScan configuration the 1375nm cannot be fully tested. Therefore, two different CropScan spectral bands were used to validate the model.

The wavelengths used were 1050nm and 1650nm, which were positioned on the NIR vegetation reflectance plateau and in the SWIR region respectively. The VDB spectra were following the regression line much better than the unimproved NDVI models. The difference between the wavelengths chosen for R_{NIR} do not have a large effect on the predictive power of the improved models. Further investigation of the output of ARTMO revealed that both combinations were usually best or second best based on the RMSE. Although the regression has definitely improved, the eventual validation shows that the estimations are not very good (Figure 13). One band combination (710nm – 1050nm) for the year 2011 does look promising (Table 6) with a $R^2 = 0.633$ and RMSEP = 10.12 μgcm^{-2}. The other predictions show either a low R^2 or high RMSEP. RMSEP is considered most important when estimating leaf chlorophyll content. It was previously seen that R^2 can be good, but this only suggests that the estimations are linearly clustered. Therefore, R^2 is not the best estimator of error in these predictions. RMSEP on the other hand gives a much better estimation of error of prediction. RMSEP calculates the difference between observed and measured and gives a result in the same unit as the estimation. The result of RMSEP is then a mean of all differences, this error is much more important for predictive models than how the estimations correlate to another (R^2). In Figure 13 it can be observed that there is a saturation effect caused by the model's inability to predict larger leaf chlorophyll contents (>80 μgcm^{-2}), which were not taken into account for PROSAIL. Furthermore, it can be seen in Figure 5 that around 60 μgcm^{-2} would be underestimated, because the VDB spectra are on the left of the regression line. This means that leaf chlorophyll contents are actually higher than the model suggests for a certain NDVI value. Therefore, the model will predict lower leaf chlorophyll values when using this simulated regression.

4.2. CVI

CVI was proposed as an index which had an enhanced sensitivity to leaf chlorophyll and was insensitive to LAI. The index would be especially effective at low LAI values. The index should fit the purpose of leaf chlorophyll estimation. The results of CVI initially looked more promising than the results of the models based on NDVI. A relation was found, but it did not fit the VDB validation spectra. The big advantage of CVI is its practicality in precision agriculture, because it uses spectral bands which are used by most agricultural monitoring systems.

The CVI showed to be insensitive to LAI at lower leaf chlorophyll contents (< 50 μgcm^{-2}). The spread of points in Figure 6 is minimal in this lower leaf chlorophyll range. CVI is designed to be insensitive to LAI (Vincini et al., 2007), which corresponds with the behaviour of CVI in this research. However, CVI appears to become more sensitive to LAI at higher leaf chlorophyll contents. Kooistra & Clevers (2016) found with ANOVA analysis on a simulated dataset with PROSAIL that CVI explained variation in leaf chlorophyll content rather poorly (60.3%) and that this variation is explained more by LAI (16.3%) compared to other ratio indices used. This could suggest that at higher leaf chlorophyll content the effects of LAI become stronger, resulting in more spread and sensitivity to LAI. In Figure 6 it can also be seen that CVI is rather insensitive to leaf chlorophyll. The points in the scatterplot at lower levels of leaf chlorophyll are plotted on top of each other. This means that with increasing leaf chlorophyll content the CVI value does not change. This insensitivity was not expected and was not found in previous research (Vincini et al., 2007, 2008; Vincini & Frazzi, 2009, 2011). Their research usually used a limited range of leaf chlorophyll content and no or a small range of LAD values. A reason for this could be the crop, because potato was not investigated in these previous works. However, at higher leaf chlorophyll content the CVI does become more sensitive to leaf chlorophyll content, which corresponds with Vincini et al. (2014). Similarly to the models based on NDVI the large range of LAD had no effect on the outcome of the PROSAIL model.

The results showed no difference in performance of the models based on the different sensors. The CVI required three spectral bands which were positioned in the R_{GREEN}, R_{RED} and R_{NIR}. Sentinel-2 and VENµS both have spectral bands which are attributed to these regions. Figure 6 showed that the best fit through the modelled points was a logarithmic fit ($R^2_{Sentinel\text{-}2} = 0.77$ and $R^2_{VEN\mu S} = 0.76$). A linear fit was also sufficient ($R^2_{Sentinel\text{-}2} = 0.62$ and $R^2_{VEN\mu S} = 0.62$) which were similar results to the performance of the regression found in Kooistra & Clevers (2016) ($R^2 = 0.64$). The small difference is due to the high R^2 for the sampled year 2014 ($R^2_{2014} = 0.84$), which was not included in this research.

Validating the proposed model based on CVI showed that the model would not be able to properly predict the leaf chlorophyll content of the VDB spectra. A logarithmic fit was created through the modelled leaf chlorophyll content, however, the VDB spectra are located on the left side of the regression curve (Figure 7). This means that for the VDB spectra much lower values are calculated at higher leaf chlorophyll content. This does suggest that there is a relation between the VDB spectra and leaf chlorophyll concentration, because there appears to be a linear relation. In Figure 14 this linear relation is presented more clearly. The logarithmic regression built with the PROSAIL model based on CVI always underestimates the actual measured leaf chlorophyll content in the VDB spectra. However, there is potential for an empirical linear relation instead of using the simulated relationship based on PROSAIL. Table 7 shows that for all sampled years except 2013 the R^2 is quite good for both sensors. This relation has not been further explored, because it was not within the scope of this research to attempt a purely statistical approach to create empirical models.

4.3. TCARI/OSAVI

The most promising of the indices chosen was TCARI/OSAVI. The index was designed to be used for leaf chlorophyll content estimations, because it follows the idea of correcting for LAI in a reflectance signal, by dividing an index sensitive to canopy chlorophyll by an index sensitive to LAI. TCARI/OSAVI is less practical than CVI, because it is constructed as a more complex ratio index compared to CVI. The spectral bands in TCARI/OSAVI cannot be chosen as 'freely' as in CVI, because of its theoretical base. Information of four spectral bands is required to use this spectral index, of which two are located in the Red-Edge spectral region. Therefore, spectral band selection was expected to have a large effect on the performance of the models based on TCARI/OSAVI.

TCARI/OSAVI performed well under the initial PROSAIL parameters as presented by Table 1. The index was insensitive to LAI at higher leaf chlorophyll contents and more sensitive to LAI at lower leaf chlorophyll contents (Figure 8). At 70-80 μgcm^{-2} the sensitivity analysis showed that the model was also insensitive to leaf chlorophyll change, but the insensitivity was not as strong as for the model built based on CVI. At lower leaf chlorophyll content more variation can be observed. A specific area can be seen in the bottom left of both plots in Figure 8 as described in Section 3.1.3. This particular spread will be explained below. As Haboudane et al. (2002) acknowledge in their research the sensitivity of TCARI to LAI increases in early growth stages of vegetation, which can be related to low leaf chlorophyll content. By combining with OSAVI this effect is drastically reduced. However, the index still shows some sensitivity to LAI at lower leaf chlorophyll content. The same is found in the results of this research. However, the index performs much better than the other indices concerning LAI sensitivity, which was also found by Wu et al. (2008). For further prediction of leaf chlorophyll these models are not yet applicable.

The spectral band definition of TCARI/OSAVI was not as 'free' as the other two indices. This means that TCARI and OSAVI are both defined by carefully calculated ratios between indices (Kim, Daughtry, Chappelle, McMurtrey, & Walthall, 1994; Rondeaux, Steven, & Baret, 1996). Because both sensors possessed relevant spectral bands to be used for TCARI/OSAVI no real differences were found between both sensor (Figure 8). An exponential fit is found for both models based on the different sensors ($R^2_{\text{Sentinel-2}}$ = 0.60 & $R^2_{\text{VEN}\mu\text{S}}$ = 0.60), which was also found by Wu et al. (Wu et al., 2008). Haboudane et al. (2002) and Kooistra & Clevers (2016) found that TCARI/OSAVI was logarithmically related to leaf chlorophyll content. The logarithmic fit in Figure 8 scores almost as well as the exponential fit ($R^2_{\text{Sentinel-2}}$ = 0.58 & $R^2_{\text{VEN}\mu\text{S}}$ = 0.58).

As mentioned before, there was a small divergence of spread in Figure 8 which was caused by the extreme range in LAD. To improve these models based on TCARI/OSAVI the PROSAIL parameter LAD was constrained to a more realistic LAD range (Section 2.2.2.2). The improvement had a positive effect on the results of these models (Figure 9). Apparently TCARI/OSAVI is sensitive to LAD at lower leaf chlorophyll content. This suggests that for field measurements LAD has to be taken into account for prediction of leaf chlorophyll. The performance of TCARI/OSAVI was now comparable to Haboudane et al. (2002) (R^2 = 0.98), Wu et al. (Wu et al., 2008) (R^2 = 0.88) and Kooistra & Clevers (2016) (R^2 = 0.88).

Validation with the VDB data showed that a good model was built for both sensors (Figure 10 and Figure 11). It is important to note that the VDB spectra do not have low leaf chlorophyll content, so the model was not validated for low leaf chlorophyll content. The VDB spectra seem to be linearly correlated with leaf chlorophyll content (Table 8), but this linearity can also be observed in Figure 9 at higher leaf chlorophyll content (> 40 μgcm^{-2}) in the model. At this higher leaf chlorophyll content it was assumed that TCARI/OSAVI was insensitive to leaf chlorophyll and LAI. The VDB spectra are located within the parameter variation of the results of the PROSAIL model (Figure 11). It could be that the VDB spectra would be better fitted with the PROSAIL model if the leaf chlorophyll parameter had a larger range. The results are also slightly affected by the spectral band differences between the spaceborne sensors (Sentinel-2 and VENµS) and CropScan. In Figure 15 the outcome of the leaf chlorophyll predictions are plotted. Both models based on TCARI/OSAVI are able to predict leaf chlorophyll well (RMSEP < 10 μgcm^{-2}), except for the sampled year 2010 (Table 8). The sampled year 2010 was addressed in Section 4.1. In Figure 15 an underestimation similar to the underestimations made by the models based on NDVI can be observed. This is again most likely due to the model's inability to properly predict leaf chlorophyll content over 80 μgcm^{-2}.

5. Conclusion

TCARI/OSAVI was the best vegetation index for predicting leaf chlorophyll content from canopy spectra after constraining the LAD parameter. Sensitivity analysis with PROSAIL in ARTMO showed that TCARI/OSAVI was insensitive to LAI, which made it a capable vegetation index to estimate leaf chlorophyll from canopy (crop) spectra using radiative transfer modelling. The computing power of ARTMO opened up many possibilities for radiative transfer modelling, where a lot of parameters and ranges of parameters could be varied.

Spectral band definitions had different effects per sensor. NDVI was affected by choosing different spectral bands, which gave cause to the improved ‘pseudo’ NDVI. CVI was much less affected by different spectral band definitions as was TCARI/OSAVI. However, TCARI/OSAVI required specific spectral bands which could not easily be varied in the sensitivity analysis. The relationship between leaf chlorophyll content and a vegetation index differed per vegetation index. TCARI/OSAVI had the best relationship with leaf chlorophyll content, which has also been confirmed by other works. It is acknowledged that the relationship of CVI has to be further explored as there appears to be a linear relationship, but it could not be explained by the PROSAIL model.

Two improvements were applied to the models initially created by PROSAIL. Best Band combination had a large effect on the performance of the models based on NDVI. It changed the relationship of an inaccurate exponential model to a rather accurate linear model. The spectral band definition changed from a RED and NIR band to a Red-Edge and water sensitive band, as related index of the NDWI, but this relationship has to be explored further. CVI was not improved by using either method (Best Band combination & Constraint), but as mentioned before it could be improved with empirical analysis of the linear relationship found. TCARI/OSAVI was greatly improved by constraining the LAD parameter in PROSAIL. By doing so, the accuracy of the PROSAIL models based on TCARI/OSAVI increased to the point that these models could be used for leaf chlorophyll estimation.

6. Recommendations

ARTMO proved to be very capable of performing sensitivity analysis. Not only by doing RTM, but it also contains MLA and other powerful statistical procedures. These were not explored in this research. However, it is strongly recommended to explore these methods, as they could increase the effectiveness of RTM and sensitivity analysis of vegetation indices. It was also possible in ARTMO to create models for every nanometer in the spectrum. Considering the interesting finding of the ratio index which resembled the NDWI, this could provide more possibilities for undiscovered vegetation indices.

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8. Appendix

Table 9: CropScan specifications

SPECTRAL BAND POSITION (NM)	BANDWIDTH (NM)
490	7.3
530	8.5
550	9.2
570	9.7
670	11
700	12
710	12
740	13
750	13
780	11
870	12
940	13
950	13
1000	15
1050	15
1650	200

Table 10: Sentinel-2 specifications

BAND NAME	MIN	MAX	CENTER	FWHM
BAND1	433.000	453.000	443	20
BAND2	457.500	522.500	490	65
BAND3	542.500	577.500	560	35
BAND4	650.000	680.000	665	30
BAND5	697.500	712.500	705	15
BAND6	732.500	747.500	740	15
BAND7	773.000	793.000	783	20
BAND8	784.500	899.500	842	115

BAND8A	855.000	875.000	865	20
BAND9	935.000	955.000	945	20
BAND10	1360.000	1390.000	1375	30
BAND11	1565.000	1655.000	1610	90
BAND12	2100.000	2280.000	2190	180

Table 11: VENuS specifications

BAND NAME	MIN	MAX	CENTER	FWHM
BAND1	400.000	440.000	420	40
BAND2	423.000	463.000	443	40
BAND3	470.000	510.000	490	40
BAND4	535.000	575.000	555	40
BAND5	600.000	640.000	620	40
BAND6	652.000	682.000	667	30
BAND7	690.000	714.000	702	24
BAND8	734.000	750.000	742	16
BAND9	774.000	790.000	782	16
BAND10	845.000	885.000	865	40
BAND11	900.000	920.000	910	20