Multi-Angle Spectroscopic Remote Sensing of Arctic Vegetation Biochemical and Biophysical Properties

By

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Abstract

Estimating the spatial distribution of foliar pigments and canopy structural components with remote sensing can serve as an important approach for monitoring plant community characteristics, as spatially explicit measurements of vegetation biochemical and biophysical variables can provide insight into ecosystem composition, processes, and/or disturbance caused by changing environmental conditions. Vegetation monitoring efforts in Arctic regions have been mostly accomplished with nadir-looking broadband instruments, thus leaving multi-angle, spectroscopic retrievals of vegetation biochemical and biophysical variables largely unexplored.

Using field and spaceborne (CHRIS/PROBA) multi-angle spectroscopy, the performance of various modelling techniques was compared for retrieving biochemical and biophysical variables from tundra vegetation situated across a bioclimatic gradient in the Western Canadian Arctic. Specifically, empirically-based multi-band and predefined narrowband vegetation indices (VIs), a machine learning regression algorithm (Gaussian processes regression, GPR), and a physically-based radiative transfer model (PROSAIL) were compared for their capability of retrieving leaf chlorophyll content (LCC), plant area index (PAI), and canopy chlorophyll content (CCC) from multi-angle, multi-scale, high-resolution canopy reflectance data. Reference data for these variables were acquired through laboratory and field-scale leaf and canopy measurements.

Iterative empirical models were the most effective for retrieving LCC, PAI, and CCC irrespective of view angle and spatial scale ($p \leq 0.05$). GPR produced the best correlation-based modelling results (cross validated $r^2_{cv}=0.59$), however, a multi-band vegetation index (i.e. simple ratio, SR) was shown to provide statistically comparable results while providing a more simplistic methodological approach ($r^2_{cv}=0.55$). Furthermore, SR produced statistically superior ($p \leq 0.05$) normalized prediction accuracies over GPR (NRMSE=0.13 vs. NRMSE=0.16). Empirically

modelled band selections showed that variable covariation is an important consideration when constructing reflectance models used for vegetation variable retrievals in the Arctic, and thus it was concluded that spectroscopic remote sensing provides benefits for such tasks. The overall conclusion drawn from the compiled empirical and physical modelling results, when examined across the field and remote sensing scales, was that a multi-angle approach does not provide a statistically significant advantage over a nadir approach for retrieving LCC, PAI, or CCC in Arctic environments ($p>0.05$).

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List of Acronyms

ACM	Atmospheric correction module
ALA	Average leaf angle
ALA_e	Effective average leaf angle
ALA_t	True average leaf angle
ANN	Artificial neural network
ANOVA	Analysis of variance
AOT	Aerosol optical thickness
ARI	Aurora Research Institute (Inuvik, Northwest Territories, Canada)
ARTMO	Automated Radiative Transfer Models Operator
ASD	Analytical Spectral Devices FieldSpec handheld spectroradiometer
ASL	Above sea level
AVHRR	Advanced Very High Resolution Radiometer
B1	Band 1
B2	Band 2
BAT	Band Analysis Tool
BGI	Blue green (vegetation) index
BRDF	Bidirectional reflectance distribution function
BRF	Bidirectional reflectance factor
<i>C_{ab}</i>	Chlorophyll <i>a+b</i> (leaf chlorophyll content)
<i>C_{ar}</i>	Carotenoids (leaf carotenoid content)
CAVM	Circumpolar Arctic Vegetation Map
<i>C_{bp}</i>	Leaf brown pigment content
CCC	Canopy chlorophyll content
CCC_e	Effective canopy chlorophyll content
CHRIS	Compact High Resolution Imaging Spectrometer
<i>C_m</i>	Leaf dry matter content
COI	Circle of interest
<i>C_w</i>	Equivalent water thickness
CWV	Columnar water vapour

DEM	Digital elevation model
DHP	Downward hemispherical photography
DW	Dry (leaf) weight
EnMAP	Environmental Mapping and Analysis Program
EVI	Enhanced vegetation index
EWT	Equivalent water thickness
<i>f</i>APAR	Fraction of absorbed photosynthetically active radiation
<i>f</i>Cover	Fraction of vegetation cover at nadir
FMC	Full moisture content
FOV	Field of view
FW	Fresh (leaf) weight
FWHM	Full width at half maximum
GCP	Ground control point
GFOV	Ground field of view
GOA	Greening of the Arctic
GPP	Gross primary productivity
GPR	Gaussian processes regression
GPR-BAT	Gaussian Processes Regression - Band Analysis Tool
GPS	Global positioning system
GVI	Green vegetation index
IFOV	Instantaneous field of view
ISODATA	Iterative Self-Organizing Data Analysis Technique
JPEG	Image format (Joint Photographic Experts Group)
KRR	Kernel ridge regression
LAD	Leaf angle distribution
LAI	Leaf area index
LAI_e	Effective leaf area index
LAI_t	True leaf area index
LCC	Leaf chlorophyll content
LMA	Levenberg-Marquardt algorithm
LUE	Light use efficiency

LUT	Look-up-table
M1	CHRIS/PROBA Mode-1
MAAT	Mean annual air temperature
MISR	Multi-angle Imaging Spectrometer
MLRA	Machine learning regression algorithm
MODIS	MOderate Resolution Imaging Spectrometer
MODTRAN	MODerate resolution TRANsmittance
<i>N</i>	Leaf structure parameter
NDVI	Normalized difference vegetation index
NIR	Near-infrared
nm	Nanometer
NPP	Net primary productivity
NRMSE	Normalized root mean square error
NRMSE_{cv}	Cross-validated normalized root mean square error
NT	Northwest Territories, Canada
OSAVI	Optimized soil adjusted vegetation index
PAI	Plant area index
PAI_d	Destructive plant area index
PAI_e	Effective plant area index
PAI_t	True plant area index
pH	Potential of hydrogen
PLSR	Partial least squares regression
PROBA	Project for On Board Autonomy
PROSAIL	Combination of PROSPECT-5 and SAILH radiative transfer models
PROSPECT	A model of leaf optical properties spectra (leaf radiative transfer model)
<i>P_s</i>	Soil reflectance parameter
QUAC	QUick Atmospheric Correction
<i>r</i>²	Coefficient of determination
<i>r</i>²_{cv}	Cross-validated coefficient of determination
RAA	Relative azimuth angle
RAMI	RAdiative transfer Model Intercomparison

RE	Relative error
RE	Red-edge (wavelength region)
RFE	Recursive feature elimination
RMCARI	Revised modified chlorophyll absorption ratio index
RMSE	Root mean square error
RMSE_{cv}	Cross-validated root mean square error
ROSAVI	Revised optimized soil adjusted vegetation index
RTM	Radiative transfer model
RUE	Radiation use efficiency
RVM	Relevance vector machines
SAA	Sun azimuth angle
SAIL	Scattering by Arbitrarily Inclined Leaves (canopy radiative transfer model)
SAVI	Soil adjusted vegetation index
SBBR	Sequential backward band removal
<i>SKYL</i>	Ratio of diffuse to total incident radiation
<i>S_L</i>	Hot spot parameter
SLR	Single lens reflex (camera)
SMLR	Stepwise multiple linear regression
SPAD	Minolta SPAD-502 leaf chlorophyll meter
SR	Simple ratio (vegetation index)
SRF	Spectral response function
SVM	Support vector machines
SVR	Support vector regression
SWIR	Short-wavelength infrared (wavelength region)
SZA	Solar zenith angle
TOA	Top of atmosphere
TOC	Top of canopy
TRAC	Tracing Radiation and Architecture of Canopies
TSAVI	Transformed soil adjusted vegetation index
USA	United States of America
VAA	View azimuth angle

VI	Vegetation index
VIS	Visible (wavelength region)
VNIR	Visible near-infrared (wavelength region)
VZA	View zenith angle
WGS 84	World Geodetic System 1984
YT	Yukon Territory, Canada

PART I: Introduction and Background

Chapter 1. Introduction and Objectives

1.1. Introduction

The Arctic is experiencing dramatic environmental changes that are expected to have profound impacts on Arctic ecosystems (ACIA, 2005; CAFF, 2013). Average annual Arctic temperatures have risen by ~ 2 °C since the 1950s, the observed warming being the greatest over land areas (Chapman & Walsh, 2003; Chapin et al., 2005; Hinzman et al., 2005; Overland et al., 2002). This has resulted in extensive melting of glaciers (Sapiano et al., 1997), increases to hydrologic variability (Smith et al., 2005), thawing of permafrost (Osterkamp, 1994), increased active layer depth (Mack et al., 2004; Van Wijk et al., 2004), and reduction in extent of sea ice (Rothrock et al., 1999; Vinnikov et al., 1999). These documented environmental changes not only alter existing plant growth and ecosystem balance over the short term, but have the potential to affect competitive interactions between species that can result in changes in vegetation composition and climate over the long term (Sturm et al., 2001; Huemmrich et al., 2010a,b).

Ecosystem responses to warming have the potential to feedback either positively or negatively to the climate system depending on changes in the vegetation distribution and productivity (Goetz et al., 2011; McGuire et al., 2009). For example, northward advance of the tree line results in short tundra vegetation being replaced by trees and forest, thereby reducing surface albedo and producing a positive feedback on temperature (Bala et al., 2007; Chapin et al., 2005; Randerson et al., 2006). Conversely, the associated increased productivity of Arctic vegetation tends to result in increased carbon dioxide uptake by net photosynthesis, theoretically providing a negative feedback to rising temperatures (Goetz et al., 2011; Field et al., 2007; Serreze et al., 2000). Both

photosynthetic and respiratory processes (i.e. greening) can be stimulated by warming (Oberbauer et al., 2007) and the balance of these processes has an influence on such things as the net carbon flux (Huemmrich et al., 2010a,b). The relative importance of competing feedbacks, and thus the cumulative effect of changing Arctic vegetation on the climate system, is still not well known (McMichael et al., 1999; Muller et al., 1999; Walker, 2000; Stow et al., 2004; Gamon et al., 2013), primarily because of the vast areas ($\sim 5 \times 10^6 \text{ km}^2$) and different vegetation types involved, most of which are rather inaccessible (Walker et al., 2005; Gamon et al., 2013).

In the short term, it is valid to assume that climate induced changes to vegetation structure and function in the Arctic will be expressed through changes to vegetation phenology, species assemblages, productivity (i.e. greening), and species ranges (Callaghan et al., 2004; Prowse et al., 2009; Chapin et al., 2005; Stow et al., 2004; Welker et al., 2000; Laidler et al., 2008). Indeed, changes in relative dominance of plant species have already been observed with respect to shrub intensification and the northward expansion of the tree line (Post et al., 2009; Sturm et al., 2001; Myers-Smith et al., 2011; Fraser et al., 2014a,b; Olthof & Fraser, 2014). Seasonal changes, such as warming in springtime and extended autumn warming have caused earlier melting of snow cover and later onset of winter, respectively, lengthening the growing season and increasing opportunities for plant growth (Lafleur & Humphreys, 2007; Lafleur et al., 2001; Oberbauer et al., 1998; Piao et al., 2008). Satellite observations (Bhatt et al., 2010; Goetz et al., 2005; Myneni et al., 1997) suggest that longer growing seasons (earlier onset) and enhanced greening are already occurring in various Arctic regions, supporting the hypothesis of greater vegetation production under longer snow-free growing seasons (e.g. Bhatt et al., 2010; Goetz et al., 2005; Myneni et al., 1997); however, the results of Gamon et al. (2013) and other Arctic field studies (Humphreys & LaFleur, 2011) contradict this hypothesis and instead demonstrate that greening is not necessarily

correlated with snow melt timing but other environmental conditions and their timing (e.g. precipitation, soil moisture, and growing degree days). This demonstrates the need for a diversity of enhanced techniques and methodologies for monitoring and investigating such phenomena.

Currently, monitoring Arctic vegetation change poses two major challenges. (1) Arctic landscapes are characterized by multiple scales of spatial heterogeneity, where vegetation assemblages can vary over scales ranging from centimeters to kilometers (Stow et al., 2004; Laidler et al., 2008; McFadden et al., 1998). Spatial heterogeneity and species diversity makes it difficult to apply universal modelling and retrieval approaches for monitoring. (2) Although small-scale plot-based vegetation studies may provide highly detailed local information, the climate and the remote location of field sites make such studies logistically constrained and impractical for long-term, systematic investigation and monitoring (Shippert et al., 1995; Jacobsen & Hansen, 1999) at ecosystem or landscape scales (Dungan, 1998; Lobo et al., 1998; Ostendorf & Reynolds, 1998). If implemented, small scale plot-based studies would need to be deployed across bioclimatic gradients in numerous locations representative of the biosphere in question (Gamon et al., 2013; Walker et al., 2011; Walker et al., 2016).

Remote sensing can provide more extensive spatial and temporal coverage and has the potential to improve vegetation attribute estimation precision and accuracy over larger areas, specifically through leaf and canopy biochemical and biophysical variable retrievals. It can be used for the retrieval of common vegetation variables or characteristics that span all species, which are a function of their health and physiological condition, and that are not impacted by regional spatial heterogeneity or species diversity (e.g. leaf and canopy biochemistry).

1.1.1. Imaging spectroscopy and its use in vegetation variable estimation

One of the most advanced optical remote sensing techniques used in vegetation modelling is imaging spectroscopy or hyperspectral remote sensing, which started in the early 1980s (e.g., Goetz et al., 1985) and has developed since then to include several airborne sensors and a small number of satellite sensors. It involves the measurement, quantification, and interpretation of reflectance spectra acquired in image format from an airborne or satellite sensor (Plaza et al., 2009). As it is the primary data type of this research, it is briefly introduced here in the context of its potential for vegetation variable estimation in the Arctic; additional background detail is given in Chapter 2. Imaging spectrometers used for vegetation research typically record the electromagnetic spectrum from approximately 400 nm to 2500 nm in many spectral bands (e.g., 50 to over 200 bands) with spectral sampling resolutions between 2 nm and 10 nm (Plaza et al., 2009). The value of using imaging spectroscopy lies in its ability to provide a high-resolution, contiguous reflectance spectrum for each element in the image (Jensen, 2005). Since many materials have diagnostic absorption and reflectance features that are only 10 nm to 20 nm wide, spectroscopic sensors often have sufficient spectral resolution for the direct identification of those materials based on the shape and magnitude of their associated spectra (Jensen, 2005).

Multi-angle imaging spectroscopy is defined as the near-simultaneous acquisition of spatially co-registered images in many spectrally contiguous bands, at various observation and illumination angles (Schaepman, 2007). It exploits the reflectance anisotropy of the Earth's surface that is described by the bidirectional reflectance distribution function (BRDF), which depicts the angular distribution of spectral radiation scattered by a surface (Nicodemus et al., 1977). Where traditional remote sensing applications have mostly focused on extracting structural and biochemical information from the spectral domain, multi-angle sensors take advantage of both the spectral and

angular domains (Chopping, 2008). Spectro-directional observations have been shown to significantly improve the quality and reliability of reflectance-based vegetation variable estimates (Diner et al., 1999; Rast et al., 2001, Rast et al., 2004; Meneti et al., 2005; Diner et al., 2005; Schaepman, 2007; Verrelst et al., 2008; Stagakis et al., 2010; Sykioti et al., 2011; Hilker et al., 2011; Hilker et al., 2017).

Multi-angle space-borne imaging spectrometers have been operational, including the Compact High Resolution Imaging Spectrometer (CHRIS) sensor (used in this research) onboard the Project for On-Board Autonomy (PROBA) platform (CHRIS/PROBA) (Barnsley et al., 2004) and the Multi-angle Imaging Spectrometer (MISR) (Lucht, 1998), while future missions include EnMAP (Environmental Mapping and Analysis Program) (Kaufmann et al., 2006). In this thesis, multi-angle reflectance anisotropy is analyzed at both the field and satellite scales to determine its utility in vegetation variable retrieval.

Imaging spectrometers are increasingly being used to measure the pigment (e.g. chlorophyll, carotenoids, and anthocyanins) and non-pigment (e.g. nitrogen, carbon, lignin, cellulose, and water) biochemical constituents of vegetation (Ustin et al., 2004; Blackburn, 2007; Ustin et al., 2009). Quantifying foliar and canopy biochemical constituents is of great interest because of the important role they play in physiological processes such as photosynthesis, their relationship with ecosystem processes such as litter decomposition and nutrient cycling, their use for identifying plant species and functional groups, and their use for assessing plant/ecosystem stress (Schaepman et al., 2009; Ustin et al., 2009; Kokaly et al., 2009). Accurate remotely-sensed estimates of foliar biochemical concentrations can therefore provide a valuable aid to understanding ecosystem composition and functioning over a wide range of environments and spatio-temporal scales (Schaepman et al., 2009). For example, chlorophyll, also considered a measure of land surface

greenness, has been shown to be correlated with leaf area index (LAI) or plant area index (PAI, as used in this thesis includes green vegetation components), leaf and plant canopy photosynthetic radiation use efficiency (RUE), and gross primary production (GPP) (Curran et al., 1990; Gitelson et al., 2006; Tucker, 1979; Asrar et al., 1984; Tucker & Sellers, 1986; Myneni et al., 1995; Zhou et al., 2003, Garrity et al., 2011), and is therefore useful for studies concerning the spatial distribution of plants and their seasonal functioning (Stitch et al., 2007). Chlorophyll distribution in vegetation is strongly related to leaf nitrogen content (Daughtry et al., 2000) and responds to plant disturbance and stress, thus acting as a bio-indicator of plant physiological condition (Gitelson et al., 2003; Sampson et al., 2003; Zarco-Tejada et al., 2002). Chlorophyll is also linked to carbon and nitrogen cycles and its role in photosynthesis and net primary productivity (NPP) is important within regional and global carbon models and related climate feedbacks (Inoue, 2003; Croft et al., 2013; Knyazikhin et al., 2013a,b; Heimann & Reichstein, 2008).

In addition to monitoring the biochemical aspects of vegetation, imaging spectroscopy has also been shown to provide enhanced means of characterizing the biophysical-structural aspects of vegetation canopies (Darvishzadeh et al., 2008a; Borzuchowski & Schulz, 2010; Stagakis et al., 2010; Sykioti et al., 2011; Li et al., 2014a; Verrelst et al., 2015a,b). For example, the quantification of LAI from remote sensing data can provide an understanding of dynamic changes in ecosystem productivity and be used as an indicator for climate related impacts on ecosystems (Zheng & Moskal, 2009). Remotely-sensed measurements of LAI are therefore an important component to monitoring and modelling of ecological variables and processes both spatially and temporally (Green et al., 1997; Liu et al., 1997; Zheng & Moskal, 2009). In addition, retrievals of LAI can be used to up-scale estimates of leaf-level biochemical constituents to the canopy for further assessment and retrieval (Darvishzadeh et al., 2008a,b; Verrelst et al., 2015a; Peng et al., 2017;

Clevers et al., 2017). Knyazikhin et al. (2013a,b) showed that canopy structure is a dominant factor in reflectance, and understanding the multiple-scattering process is critical for extracting biochemical estimates at the canopy scale.

Retrieval of vegetation biochemical and biophysical variables from imaging spectroscopy has proven successful in numerous applications and studies, such as: mapping canopy stress (Ustin et al., 1998; Suarez et al., 2008; Omari et al., 2013), mapping biochemical concentrations/quantities (Townsend et al., 2003; Darvishzadeh et al., 2008a,b; Stagakis et al., 2010; Sykioti et al., 2011; Verrelst et al., 2015a; Verrelst et al., 2016), mapping vegetation composition and species dominance through biochemical variability (Asner et al., 2008a; Kokaly et al., 2003), characterizing spatial patterns of nutrient cycling across landscapes (Smith et al., 2002, Ollinger et al., 2002, Siciliano et al., 2008), understanding dynamics of vegetation and ecosystem biochemistry in relation to photosynthetic efficiency (Nakaji et al., 2006; Huemmrich et al., 2010a,b; Garrity et al., 2011), and mapping canopy structural aspects (Darvishzadeh et al., 2008a,b; Stagakis et al., 2010; Sykioti et al., 2011; Verrelst et al., 2015a; Verrelst et al., 2016). However, retrieval of quantitative estimates of vegetation biochemical and biophysical constituents from space-borne imaging spectroscopy has not been conducted for Arctic tundra ecosystems. This research was designed to determine the usefulness of imaging spectroscopy for retrieving these variables, specifically chlorophyll and PAI, in northern ecosystems.

1.1.2. Field spectroscopy in the Arctic for vegetation classification and variable estimation

Despite the lack of remotely-sensed spectroscopy studies in the Arctic, field spectroscopy investigations have been numerous (Liu et al., 2017; Bratsch et al., 2016; Buchhorn et al., 2013; Davidson et al., 2016; Hope et al., 1993; Huemmrich et al., 2013; Kushida et al., 2009, 2015; Laidler et al., 2008; Riedel et al., 2005a,b; Ulrich et al., 2009). They can be broken down into two

broad categories: (1) classification-based assessments and (2) vegetation parameter/variable retrievals. Classification studies generally characterize the spectral features of different tundra vegetation types and their spectral separability (Buchhorn et al., 2013; Davidson et al., 2016; Huemmrich et al., 2013; Urich et al., 2009; Bratsch et al., 2016; Liu et al., 2017). With respect to vegetation retrievals, most Arctic-based field spectroscopic studies have focussed on correlating some sort of transformation of reflectance (e.g. vegetation indices, VIs) with a field-measured biophysical vegetation variable such as percent vegetation cover (Kushida et al., 2009; Laidler et al., 2008; Liu et al., 2017), biomass (Kushida et al., 2009; Kushida et al., 2015; Riedel et al., 2005a,b; Buchhorn et al., 2013), and LAI (Riedel et al., 2005a,b; Williams 2005; Williams et al., 2008). In studies by Buchhorn et al. (2013) and Liu et al. (2017), narrowband VIs were found to perform better than broadband VIs in modelling of green vegetation cover and biomass, respectively. Regarding the estimation of leaf and canopy biochemistry, there are fewer studies. One example is Huemmrich et al. (2013), who correlated light use efficiency (LUE) calculated from functional type cover fractions with a 3-band hyperspectral VI used as a proxy for chlorophyll concentrations (no actual chlorophyll measurements were taken in the field). No studies have used field spectroscopy for the retrieval of vegetation biochemical variables such as leaf chlorophyll content (LCC) and canopy chlorophyll content (CCC) in the Arctic, and no studies have incorporated multi-angle field spectroscopy for retrieval of vegetation variable estimates. This research was designed to address both gaps in current and past Arctic vegetation research.

1.1.3. Vegetation variable retrieval methods

Besides the measurement of reflectance spectra, the modelling methods used to retrieve vegetation variables using spectroscopic data also play an important role in the quality of the estimated values; they must be flexible and robust (Zhao et al., 2013). These methods can be

broken down into two broad categories: (1) empirically based parametric and non-parametric regression methods (Darvishzadeh et al., 2008a; Zhao et al., 2013; Verrelst et al., 2015a,b; Verrelst et al., 2016) and (2) physically-based radiative transfer modelling (RTM) methods (Darvishzadeh et al., 2008a,b; Jacquemoud et al., 2009; Verrelst et al., 2015a,b). Both have been used extensively in a variety of settings and environments with various sensors (see Ustin et al., 2009; Kokaly et al., 2009; Jacquemoud et al., 2009; Darvishzadeh et al., 2008a,b; Stagakis et al., 2010; Sykioti et al., 2011; Verrelst et al., 2015a,b; Verrelst et al., 2016; Hilker et al., 2017, etc.). However, there has not been a robust comparison of these retrieval methods using either field spectroscopy or space-borne imaging spectroscopy. This thesis compares such methods, including: (1) parametric regression based on multi-band and predefined narrowband VIs, (2) non-parametric machine learning regression (Gaussian Processes Regression, GPR) (Rasmussen & Williams, 2006; Verrelst et al., 2016), and (3) a leaf and canopy RTM, PROSAIL (Baret et al., 1992; Jacquemoud et al., 2009).

1.2. Objectives and Research Questions

The goal of this research was to investigate the capability of CHRIS/PROBA for retrieving quantitative estimates of LCC, PAI, and CCC (LCC x PAI) from tundra vegetation communities situated across a bioclimatic gradient in the Western Canadian Arctic. To the knowledge of the author, at the time of writing there has not been any previous investigation into the use of multi-angle space-borne imaging spectroscopy for such retrievals in Arctic tundra vegetation. Multi-angle experiments, such as these, allow for the testing of the robustness of retrieval methods under a variety of sun/sensor geometries and environmental conditions, while alleviating any doubts over the applicability of multi-angle remote sensing in Arctic tundra ecosystems. The following major research question was developed.

- I. Can CHRIS/PROBA data be used to retrieve LCC, PAI, and CCC in Arctic environments and does multi-angular capability provide any benefit for vegetation variable retrieval over nadir view in Arctic tundra ecosystems?

Three objectives were defined representing leaf-canopy vegetation biochemical-biophysical measurement and characterization across the latitudinal gradient, field-scale retrieval of vegetation variables, and remotely-sensed retrieval of the same vegetation variables as listed below.

Objective 1, Leaf and Canopy Characterization: Characterize LCC, PAI, and CCC across each of the study sites (study sites are described in Chapter 2). These field data were used to provide model calibration and parameterization values. From this objective, several research questions were developed:

- I. What is the typical LCC that occurs across the Western Arctic and does a latitudinal gradient exist between study sites?
- II. What is the typical PAI of Arctic tundra vegetation as it exists in the Western Canadian Arctic and does a latitudinal gradient exist between sites?
- III. Can PAI be successfully measured, quickly and non-destructively using downward looking hemispherical photography?

Objective 2, Field Level Analysis and Modelling: Determine the capabilities of empirical (i.e. parametric and non-parametric regression) and physical modelling approaches for retrieving LCC, PAI, and CCC at the field scale across various geographic locations. Field spectral measurements were completed at multiple view angles to investigate the retrieval accuracies at the various expected sun/sensor geometries. From this objective, several research questions were developed:

- I. Can empirical modelling methodologies, specifically narrow-band VIs, combined with parametric linear regression, be used to retrieve LCC, PAI, and CCC at the field-level across various illumination/observation angles? Further to this, what VI provides the most robust retrieval accuracy regardless of observation angle?
- II. Can full spectrum non-linear non-parametric machine learning GPR perform better than traditional parametric linear regression based on VIs for retrieving LCC, PAI, and CCC at the field-level across various illumination/observation angles?
- III. Can the physically-based PROSAIL model be used to accurately simulate the top of canopy spectral-directional reflectance of Arctic tundra vegetation? Furthermore, can the PROSAIL model be inverted to predict LCC, PAI, and CCC at various illumination/observation angles?
- IV. Does spectral and spatial resolution play a role in model outcome? Can a spectral subset be used to predict LCC, PAI, and CCC with the same degree of precision as the full spectrum dataset when using the above modelling techniques?
- V. Finally, what are the optimal optical wavelengths for predicting LCC, PAI, and CCC across the Arctic and across multiple view angles?

Objective 3, Remote Sensing Level Modelling: Building on Objectives 1 and 2, determine the performance of the selected/optimized empirical and physical techniques tested at the field-scale in estimating the LCC, PAI, and CCC using CHRIS/PROBA multi-angular spectroscopic data. Additional to the primary questions asked, research questions at this level include:

- I. What modelling technique (empirical vs. physical) is best suited for retrieving LCC, PAI, and CCC from multi-angle CHRIS/PROBA data in Arctic environments?

- II. What are the optimal bandwidths for retrieving LCC, PAI, and CCC in the Arctic from CHRIS/PROBA data?

1.3. Thesis Structure

The thesis is divided into three parts: (I) Introduction (Chapter 1) and Background/Literature Review (Chapter 2), (II) Field and Remote Sensing Studies (Chapters 3-7), and (III) Synthesis and Conclusions (Chapter 8).

Part II is comprised of five studies, each focusing on a different scale of inquiry and each providing the basis for the subsequent level of investigation. Each chapter in Part II is written in journal article format, hence some repetition of study sites and methods was necessary, but repetitive text between chapters has been minimized. More specifically, Part II is organized as follows:

(1) Leaf and canopy level investigations were conducted to determine the biochemical and biophysical characteristics of Arctic tundra vegetation across the study areas. Furthermore, these investigations were completed to: (a) calibrate and parameterize the empirical and physical modelling approach, and (b) determine the efficacy of the field-based measurement techniques. **Chapter 3** provides a lab-based spectrophotometric analysis of leaf chlorophyll, carotenoids, water, and weight for various species that are typical of the Western Canadian Arctic. **Chapter 4** provides a field and lab-based characterization of canopy structure (PAI and canopy gap fractions) for each of the study sites. Canopy properties were measured using destructive techniques and then compared to modelled values derived from downward-looking hemispherical photography.

(2) Field level investigations were conducted to investigate the influence of spatial scale, spectral resampling, and sun/sensor geometry on the spectroscopic estimation of leaf and canopy

biochemical constituents and canopy biophysical properties using both empirical and physical modeling approaches. **Chapter 5** provides a comparison of parametric regression-based multi-band and pre-defined narrowband VIs with non-parametric GPR for modelling the biochemical and biophysical variables. **Chapter 6** evaluates the PROSAIL RTM (and its inversion) for predicting the leaf and canopy vegetation variables and parameters. PROSAIL inversion was completed using a robust non-linear least squares curve fitting algorithm, also known as the Levenberg-Marquardt least squares minimization algorithm (LMA).

(3) Remote sensing level investigations were conducted to determine whether the biochemical and biophysical variables investigated at the field/plot scales could be estimated using medium resolution space-borne imaging spectroscopy in conjunction with the optimal modeling approaches used at the field scale. **Chapter 7** investigates the use of CHRIS/PROBA for retrieving LCC, PAI, and CCC using VIs, MLRAs, and RTM and inversion. Lessons learned at the field scale are applied to the remote sensing scale.

Part III provides a synthesis of the overall statistical and qualitative analysis of the field and remote sensing studies leading to conclusions with respect to the major questions: (1) is multi-angle data useful and if so, which view zenith angle is best for retrieval of the various vegetation variables, and (2) which modelling approach provides the best overall results irrespective of look angle.

Chapter 2. Study Area and Methodological Approach

2.1. Study Area and Image Acquisitions

The study sites selected for this research are situated across the Western Canadian Arctic within the Northern and Southern Arctic and Taiga Cordillera Terrestrial Ecozones (ESWG, 1995). Satellite and historical records (ground-based photographs and plot-based studies) of vegetation in the region provide evidence of enhanced greening (i.e. vegetation growth) (Bhatt et al., 2010; Chapin et al., 2005; Sturm et al., 2001; Myers-Smith et al., 2011; Gamon et al., 2013; Fraser et al., 2014a,b; Walker et al., 2016; Pouliot et al., 2009; Olthof & Fraser, 2014). Since warming has been especially rapid in the Western North American Arctic (Chapin et al., 2005; Hinzman et al., 2005; Serreze et al., 2000; Burn & Kokelj, 2009), systemic changes in this region may be indicative of how (and how quickly) other Arctic terrestrial ecosystems will change in response to similar forcing mechanisms (Gamon et al., 2013), and therefore, this region provides (and has provided) an ideal setting for vegetation related monitoring studies and methodological investigations.

The Arctic ecoregion and its sub-classification of ecozones occupies all terrestrial areas beyond the northern limit of forests (i.e. the tree line) (Walker et al., 2016). More southerly sub-Arctic tundra conditions below the tree line coincide with the presence of mountain ranges (i.e. Richardson Mountains). Tree growth in Arctic tundra regions are limited by low temperatures, moisture limitations, and short growing seasons/number of growing degree days (Walker et al., 2016; Gamon et al., 2013). The Arctic is typified by extremely cold winters below freezing and July temperatures generally below $\sim 12^{\circ}\text{C}$ (Walker et al., 2016). Areas that are not covered by glaciers, are characterized by tundra vegetation that is mostly composed of herbaceous plants, small and dwarf-like prostrate shrubs, mosses, sedges and grasses, and lichens (Walker et al., 2005; Walker et al., 2016). Vegetation patterns across this Arctic region are strongly influenced by the

presence of the Arctic ocean and its seasonal sea ice patterns (Bhatt et al., 2010; Walker et al., 2016). Bhatt et al. (2010) provided a linkage between diminishing Arctic sea ice and increasing Arctic terrestrial ecosystem productivity (i.e. greening) in Northern Alaska and along the Beaufort Sea coastline.

At the regional scale, the diversity of plant species and the morphological forms of Arctic species is related to the summer mean air temperatures found along latitudinal and altitudinal gradients (CAFF, 2013; Walker et al., 2016). As such, species diversity decreases with increasing latitude and altitude, both similarly (Daniëls et al., 2013), where altitudinal gradients are additionally affected by slope (angle and orientation), duration of snow cover, and sunlight hours (Sieg et al., 2006; Walker et al., 2016). The Arctic possesses 2218 known species of vascular plants, ~900 species of bryophytes (mosses and liverworts), and ~1750 species of lichens (Elven et al., 2011; Daniëls et al., 2013; Dahlberg and Bültmann, 2013; Walker et al., 2016).

At the landscape scale, species diversity and vegetation productivity are related to surface geology and topography (e.g. bedrock and surficial geology, geomorphology, glacial history, and permafrost), and the role that these features play on the spatial distribution of soil development and moisture regimes (e.g. snow accumulation and wetland distribution) (Walker et al., 2016). The distribution of vegetation in the Arctic has also been shown to be strongly related to soil pH (potential of hydrogen) (Edlund, 1982; Elvebakk, 1997; Walker et al., 1998; Buchhorn et al., 2013; Walker et al., 2016). The spatial variability of soil pH has been shown to affect vegetation community structure and diversity, as well as ecosystem-scale properties and processes, such as soil temperatures, active layer depth, photosynthesis rates, plant respiration, plant matter decomposition, and fluxes (e.g. gasses, water, energy) (Walker et al., 1998; Walker et al., 2016).

At fine spatial scales, vegetation distribution and vegetation assemblage/community transitions are evident along toposequences (i.e. hillslopes) and moisture gradients (i.e. wetlands) (Walker et al., 2016). Spatial variation of vegetation is also related to patterned ground features that are characteristic of all/most periglacial/permafrost regions (Washburn, 1980). Fine spatial scale variations of soil moisture and temperature in patterned ground have been shown to differ substantially within distances of a few centimeters, and in addition, vegetation biomass and thickness have been shown to affect the hydrologic, thermal, and nutrient properties of soils (Kade et al., 2005; Walker et al., 2011; Frost et al., 2013; Walker et al., 2016). The presence/absence of Arctic animal species also has an effect on the distribution and productivity patterns of tundra vegetation (Walker et al., 2016).

Figure 1 shows a map of the locations of the field sites. Following the Ecoregions of Canada framework (Ecological Stratification Working Group (ESWG), 1995), these sites include: (1) Yukon Coastal Plains (Herschel Island, YT), (2) Tuktoyaktuk Coastal Plains (Richards Island and Tuktoyaktuk, NT), (3) Banks Island Lowlands (Aulavik National Park, NT), and (4) British-Richardson Mountains, YT/NT. A diversity of field sites situated and selected across a north-south bioclimatic gradient allowed for the testing of a large range of environmental conditions and vegetation assemblages typical of each Arctic environment and thus the region. The following sections provide a brief description of each field site, including locations of the ground sampling plots and CHRIS/PROBA acquisitions. All CHRIS/PROBA imagery shown in this section has been geometrically corrected and orthorectified. Dates, acquisition angles and processing of CHRIS/PROBA are described in Chapter 7. All acquisitions are shown as true colour composites using bands 23 (red, 651 nm), 13 (green, 551 nm), and 3 (blue, 452 nm). All field campaigns were planned in accordance with imagery acquisitions and this was mostly achieved.

Figure 1 Map of the study sites situated within the Western Canadian Arctic. Map created from Atlas of Canada National Scale Data 1:1,000,000 (NRC, 2014) and Northern Geodatabase (NRC, 2012). Scale bar is approximate (as scale is variable with conical projections).

2.1.1. Yukon Coastal Plains: Herschel Island, YT

The Yukon Coastal Plains Ecoregion is situated along the Beaufort Sea, north of the British-Richardson Mountains and west of the Mackenzie River Delta (YEWG, 2004). Surface relief is low with elevations below ~30 m above sea level (ASL), though Herschel Island reaches a maximum elevation of ~185 m ASL (YEWG, 2004). Mean annual air temperature (MAAT) varies in range of -10°C to -12°C, with July mean temperatures of ~8°C to 10°C (YEWG, 2004); however, MAAT on Herschel Island has increased 2.5°C in the past century (Burn & Zhang, 2009). Mean annual precipitation is low and ranges from 125 mm to 200 mm (YEWG, 2004; Burn & Zhang, 2009). Permafrost is continuous throughout the ecoregion with soils having active layers greater than 50 cm (Burn & Zhang, 2009). Thermokarst lakes, retrogressive thaw slumps, polygons and stripes (i.e. patterned ground), lowland polygon fens/wetlands, and other periglacial features are common across much of the ecoregion (YEWG, 2004; Burn & Zhang, 2009).

On Herschel Island, the climate coupled with the large-scale physiographic features (e.g. marine environment) supports a near-continuous cover of shrubby tundra vegetation consisting of dwarf birch, alders, willows, mosses, and sedge and cotton-grass tussocks (Smith et al., 1989; Myers-Smith et al., 2011; Cray & Pollard, 2015). Recent warming on Herschel Island has resulted in the expansion of canopy-forming shrubs and an overall greening of the landscape (Burn & Zhang, 2009; Myers-Smith et al., 2011; Cray & Pollard, 2015). The flora of Herschel Island is described in detail in the vegetation survey of Smith et al. (1989). Figure 2 shows the multi-angle CHRIS/PROBA Mode-1 acquisitions for Herschel Island on July 20th, 2011. All field sampling locations/plots are displayed as red crosses. Photographs of Herschel Island (July 2011) are shown in Figure 3. All field photos demonstrate the typical vegetation condition and cover at the time of sampling.

Figure 2 Multi-angle CHRIS/PROBA M1 acquisitions for Herschel Island, YT. Field plots are indicated with a cross. Map created from Atlas of Canada National Scale Data 1:1,000,000 (NRC, 2014) and Northern Geodatabase (NRC, 2012).

Figure 3 Photographs of the ground terrain and vegetation of Herschel Island, YT. Photos taken during the July 2011 field campaign. Photographs demonstrate the typical vegetation condition and cover at the time of sampling.

2.1.2. Tuktoyaktuk Coastal Plains: Tuktoyaktuk and Richards Island, NT

The Tuktoyaktuk Coastal Plain ecoregion extends across the outer Mackenzie River Delta (Richards Island) and westward towards the Tuktoyaktuk Peninsula bordering the Beaufort Sea. The Mackenzie Delta is the largest Arctic delta in North America with a total area of ~13,000 km² (Burn & Kokelj, 2009). Much of the delta region is covered by small lakes, numbering ~25,000 with ~1200 on Richards Island alone (Lesack et al., 1991; Burn 2002). Similarly, small lakes and ponds are numerous along the Tuktoyaktuk Peninsula (~10,000) (Rampton, 1987). Permafrost is continuous in this ecoregion with active layer depths similar to those of the Yukon Coastal Plain (~50 cm) (Heginbottom et al., 1995; Burn & Kokelj, 2009). Periglacial and permafrost related processes are responsible for landforms such as thermokarst lakes, retrogressive thaw slumps, patterned ground (e.g. ice wedge polygons), lowland polygon fens/wetlands, and pingos (Burn & Kokelj, 2009). MAAT are approximately -10°C to -12°C with July mean temperatures of ~11°C (ESWG, 1995). The mean annual precipitation range is approximately 125-200 mm (ESWG, 1995). Surface relief is low with uplands reaching ~80 m ASL (Fraser et al., 2014a).

This ecoregion is characterized by a nearly-continuous cover of shrubby tundra vegetation similar to that of the Yukon Coastal Plain; however, tall shrubs (e.g. willows and alders) and stunted trees (e.g. white and black spruce) occupy warmer and more southerly sites within the tree line transition zone (Burn & Kokelj, 2009). An in-depth account of the Mackenzie Delta vegetation is provided by Burn and Kokelj (2009). Recent warming in the region has resulted in shrubification and greening of the tundra (Burn & Kokelj, 2009; Pouliot et al., 2009; Fraser et al., 2014a). Figures 4 and 5 shows multi-angle CHRIS/PROBA Mode-1 acquisitions for Tuktoyaktuk on August 3rd, 2013 and Richardson Island on August 10th, 2014, respectively. Various photographs of Richards Island and Tuktoyaktuk are shown in Figure 6. Photos were taken in July 2012 and July 2013.

Figure 4 Multi-angle CHRIS/PROBA M1 acquisitions for Tuktoyaktuk, NT. Field plots are indicated with a cross. Map created from Atlas of Canada National Scale Data 1:1,000,000 (NRC, 2014) and Northern Geodatabase (NRC, 2012).

Figure 5 CHRIS/PROBA M1 acquisitions for Richards Island, NT. Field plots are indicated with a cross. Map created from Atlas of Canada National Scale Data 1:1,000,000 (NRC, 2014) and Northern Geodatabase (NRC, 2012).

Figure 6 Photographs of the ground terrain and vegetation of Richards Island, NT and Tuktoyaktuk, NT (middle right). Photos taken in July 2012 and during the July 2013 field campaign. Photographs demonstrate the typical vegetation condition and cover at the time of sampling.

2.1.3. Banks Island Lowlands: Aulavik National Park, Banks Island, NT

Banks Island is a large island located in the western portion of the Canadian Arctic Archipelago that covers an area of $\sim 70,000 \text{ km}^2$ (French, 2017). The Banks Island Lowlands ecoregion occurs on the central portion of Banks Island and extends from north to south (ESWG, 1995). MAAT is approximately -16°C with mean July temperatures of $\sim 5^\circ\text{C}$ to 7°C (ESWG, 1995). Precipitation is low with a mean annual range of $\sim 100 \text{ mm}$ to 200 mm (ESWG, 1995). Environment Canada climate normals for Sachs Harbour (1981-2010), which is the closest permanent weather station, indicates MAAT of approximately -13°C , a mean July temperature of $\sim 7^\circ\text{C}$, and annual precipitation of $\sim 152 \text{ mm}$. Long-term climatic and environmental data are sparse for Banks Island; however, paleolimnological studies conducted in Aulavik National Park indicate that the climate is warming (Lim et al., 2008). Permafrost is deep and continuous throughout with maximum active layer depths varying between 50 and 75 cm (French, 2017). It is a lowland landscape characterized by an undulating topography with broad fluvial surfaces continually modified by weak fluvial incision and mass wasting processes (French, 2017). It is also a permafrost modified landscape containing numerous thermokarst lakes/ponds, ice-wedge polygons (i.e. patterned ground), wet sedge meadows (wetlands), and frost mounds (French, 2017).

Vegetation is often sparse and composed mainly of Arctic dwarf shrubs, mosses, grasses, sedges, and low-lying forbs/flowering plants (Larter et al., 2009; French, 2017). Vegetation zonation is controlled mainly by topography, parent materials, and drainage/moisture patterns (French, 2017). A more detailed description of the vegetation and land-cover types of Banks Island can be found in Larter and Nagy (2001) and Larter et al. (2009). Figure 7 shows multi-angle CHRIS/PROBA Mode-1 acquisitions for Banks Island for August 1st, 2012. Figure 8 shows various photographs of Banks Island in July 2012.

Figure 7 Multi-angle CHRIS/PROBA M1 acquisition for Banks Island, NT. Field plots are indicated with a cross. Map created from Atlas of Canada National Scale Data 1:1,000,000 (NRC, 2014) and Northern Geodatabase (NRC, 2012).

Figure 8 Photographs of the ground terrain and vegetation of Banks Island, NT. Photos taken during the July 2012 field campaign. Photographs demonstrate the typical vegetation condition and cover at the time of sampling.

2.1.4. British-Richardson Mountains: Richardson Mountains, YT/NT

The British and Richardson Mountains ecoregion is located south of the Yukon Coastal Plain ecoregion, running parallel to the north coast of the Yukon before trending southward, west of the Mackenzie River Delta (YEWG, 2004). The highest peaks in the ecoregion are found in the Richardson Mountains and reach above ~1600 m ASL (YEWG, 2004). Although the Richardson Mountains are not large/massive, they exert a considerable influence on the climate and weather patterns across the ecoregion (YEWG, 2004). MAAT is approximately -8°C with mean July temperatures of ~10°C (YEWG, 2004). Convective precipitation is low with a mean annual range of ~250 mm to 400 mm (YEWG, 2004) with considerable variation throughout the ecoregion. In contrast, Environment Canada climate normals for Fort McPherson (1981-2010), which is the closest permanent weather station and located at a much lower altitude (~43 m ASL), has MAAT of approximately -7°C, a mean July temperature of ~15°C, and annual precipitation of ~298 mm. Since the 1970's, MAAT have increased by 0.77°C per decade in the Western Canadian Arctic (Burn & Kokelj, 2009); however, MAAT for Fort McPherson shows a non-significant warming trend (0.034°C per year), whereas mean summer air temperatures show a non-significant cooling trend (-0.036°C per year) (Lacelle et al., 2015). Further, a significant increase in total June-July rainfall has been observed (0.31 mm per year) (Lacelle et al., 2015). The climate coupled with the vegetation supports continuous permafrost throughout the ecoregion (Harris, 1986; Heginbottom & Radburn, 1992), where gently sloping surfaces having active layer depths less than ~50 cm (Tarnocai et al., 1993). Permafrost features associated with this ecoregion include frost shattered debris, patterned ground, solifluction lobes, and thaw slumps (YEWG, 2004).

Vegetation in the Richardson Mountains is dominated by a nearly continuous cover of shrub tundra (YEWG, 2004); though, summits and upper slopes of the mountains are mostly covered

with non-vegetated rock fragments. Open spruce woodlands are common below 600 m ASL, whereas vegetation above 600 m ASL consists of dwarf shrub that transition to sub-Arctic tundra at the highest elevations (Lacelle et al., 2015; Ecosystem Classification Group, 2010; YEWG, 2004). Upper and middle slopes generally consist of dry to moist, low-shrub and heath tundra, while on lower slopes sedge tussock communities dominate (YEWG, 2004). Larger shrub thickets are common in depressions and drainage networks. A more detailed account of vegetation found in the British-Richardson Mountain ecoregion can be found in YEWG (2004).

Field sites in the Richardson Mountains were chosen due to a southerly extent and vegetation being primarily tundra, despite its more southerly geographical location. Because of the elevation of the field sites (approximately 900 m) the dominant vegetation types found at this location are typical of the more northerly field sites. This site also provided road access, a necessary convenience for the lab-based biochemical analysis. Because of the convenient access to the field site, two field seasons were completed at this location (2013 and 2014). Figure 9 shows multi-angle CHRIS/PROBA Mode-1 acquisitions for Richardson Mountains for August 2nd, 2013. Figure 10 shows multi-angle CHRIS/PROBA Mode-1 acquisitions for Richardson Mountains for July 6th, 2014. Figure 11 shows various photographs of the Richardson Mountains in July 2013.

Figure 9 Multi-angle CHRIS/PROBA M1 acquisitions for Richardson Mountains, YT/NT. Field plots are indicated with a cross. Map created from Atlas of Canada National Scale Data 1:1,000,000 (NRC, 2014) and Northern Geodatabase (NRC, 2012).

Figure 10 Multi-angle CHRIS/PROBA M1 acquisitions for Richardson Mountains, YT/NT. Field plots are indicated with a cross. Map created from Atlas of Canada National Scale Data 1:1,000,000 (NRC, 2014) and Northern Geodatabase (NRC, 2012).

Figure 11 Photographs of the ground terrain and vegetation of Richardson Mountains, YT/NT. Photos taken during the July 2013 field campaign. Photographs demonstrate the typical vegetation condition and cover at the time of sampling.

2.2. Theoretical Background and Methodological Approach

This section describes the theoretical background and methodological approach used for the retrieval of biophysical and biochemical vegetation variables at the field and remote sensing scales, focusing on the parametric regression based on VIs, non-parametric regression based on MLRAs, and physically-based RTM inversion retrieval used in all aspects of the research.

2.2.1. Monitoring Arctic environments with optical remote sensing

A major challenge to understanding Arctic ecosystem responses to rapid and long-term climate change has been the lack of continuous observations of ecosystem processes (Stow et al., 2004; Gamon et al., 2013). For that reason, there is a strong need for consistent, repeatable sampling of ecosystem properties and processes across the Arctic (Stow et al., 2004; Walker and Raynolds, 2011). Remote sensing data, available at a range of spatial and spectral resolutions on various platforms (e.g. ground-based, aerial, and spaceborne), offer considerable potential for observing and investigating the biophysical and biochemical properties of Arctic vegetation at various spatial and temporal scales (Stow et al., 2004; Gamon et al., 2013; Bartsch et al., 2016). Electro-optical satellites offer promise for large extent spatio-temporal monitoring (e.g. Advanced Very High-Resolution Radiometer, AVHRR; Moderate-Resolution Imaging Spectrometer, MODIS, and Landsat), but also present several technical difficulties that are particularly restrictive in northern latitudes. These challenges include persistent cloud cover, low sun angles/directional effects of irradiance and reflectance (Fensholt & Proud, 2012), errors arising from temporal compositing methods (Fensholt & Proud, 2012; Gamon et al., 2013), the lack of standard band definitions (Laidler et al., 2008; Buchhorn et al., 2013; Bratsch et al., 2016; Liu et al., 2017), the poor resolution of fine-scale surface features in relation to large pixel sizes (Bliss & Gold, 1994; Engstrom et al., 2005; Gamon et al., 2012; Gamon et al., 2013), the use of sensors for unintended

applications (e.g. AVHRR was not originally designed for vegetation studies) (Cracknell, 2001; Rouse et al., 1973), and the confounding effects of water and atmosphere (Stow et al., 2004; Gamon et al., 2013). These factors complicate the characterization of surface/vegetation properties, and can lead to imprecise conclusions regarding retrieval of biochemical and biophysical variables, and thus conclusions regarding the assessment of changes in vegetation cover and physiological activity.

Satellite optical remote sensing in Arctic environments appears to be somewhat in the exploratory stages with many attempts being made to establish methodological protocols and baseline vegetation inventories (e.g. Walker et al., 1995; Stow et al., 2004; Laidler et al., 2008; Gamon et al., 2013; Fensholt et al., 2012; Buchhorn et al., 2013; Liu et al., 2017; Bratsch et al., 2016; Bartsch et al., 2016; Fraser et al., 2014a; Fraser et al., 2012). In general, Arctic satellite remote sensing studies have been mostly dominated by multispectral satellite platforms that have largely focused on: (1) assessing reflectance properties of various tundra land cover types in relation to biophysical properties (e.g. biomass and LAI) (Hope et al., 1993; Riedel et al., 2005a,b; Vierling et al., 1997; Huemmrich et al. - in Stow et al., 2004; Harris et al., 2005; Rees et al., 2004); (2) mapping land cover types/units using high to coarse resolution multi-spectral data (e.g. Landsat) combined with traditional multispectral classification techniques (Schneider et al., 2009; Ulrich et al., 2009; Fraser et al., 2009; Fraser et al., 2012; Moody et al., 2014); (3) assessing tundra vegetation dynamics (e.g. phenology, net carbon exchange, response to climate change/greening/shrubification) using VIs inferred from seasonal and multi-year trends (Huemmrich et al. in Stow et al., 2004; Huemmrich et al., 2010a; Goetz et al., 2005; Jia et al., 2003; Myneni et al., 1997; Zhou et al., 2001; Bhatt et al., 2013; Gamon et al. 2013; Fraser et al., 2014a); (4) assessing the relationship between VIs, spatial resolution and vegetation cover with

high resolution imagery (e.g. IKONOS) (Laidler et al., 2008); and (5) evaluating fractional mapping approaches to estimate land cover fractions using multi-scale data (e.g. Olthof & Fraser, 2007). It is apparent from these studies and the large scale vegetation monitoring efforts (e.g. Greening of the Arctic, GOA; and the Circumpolar Arctic Vegetation Mapping efforts, CAVM) (Walker et al., 2005; Epstein et al., 2012; Walker et al., 2012) that multispectral imaging combined with VIs, such as NDVI, remains one of the most popular methods; however, varying degrees of success have been achieved in relating empirically based VIs to vegetation biophysical variables at both the field and remote sensing level (Fensholt & Proud, 2012; Stow et al., 2004; Epstein et al., 2012; Walker et al., 2012; Fraser et al., 2011; Fraser et al., 2014a).

The advantage of using VIs derived from space-borne data is their capability to enhance the vegetative signal and reduce extraneous background effects and variability (Jones & Vaughan, 2010; Jensen, 2007). This is particularly important with canopy-level remote sensing since variations in reflectance occur with atmospheric conditions, ground wetness/snow, sun angle, and reflectance from non-target features (e.g., soil, rock, woody or senesced material) (Asrar et al., 1989; Davidson & Csillag, 2001). VIs such as NDVI have often shown relatively high correlations with Arctic vegetation variables, such as biomass and LAI (Shippert et al., 1995; Walker et al., 1995); however, there is still considerable unexplained variation in the relationship between canopy variables and reflectance as measured by space-borne sensors (Fensholt & Proud, 2012; Lathrop & Pierce, 1991; Laidler & Treitz, 2003; Laidler et al., 2008). Only recently have Arctic satellite observations been directly coupled with ground observations (e.g. Bhatt et al., 2010), demonstrating that some (but not necessarily all) NDVI increases are, in fact, associated with enhanced vegetation growth (Gamon et al., 2013). It has also been shown that increased NDVI at

the time of snowmelt may be due to reduction in snow and water cover and may not indicate increased production/greening (Gamon et al., 2013).

Given the strong role remote sensing has already played in the Arctic (e.g. Stow et al., 2004; Bratsch et al., 2016), and is likely to continue to play in understanding/investigating biotic and biosphere responses to climate change, and given the technical challenges facing optical remote sensing, there will continue to be a need for (1) field-based measurements of the tundra surface that can independently validate satellite observations (Gamon et al., 2013), and (2) standardized protocols for assessing baseline vegetation biochemical and biophysical data across a multitude of sites (Walker & Raynolds, 2011). It has been suggested by Walker and Raynolds (2011) that for satellite data to be most effective in climate and ecosystem based studies, observations should be made using standardized protocols and defined biochemical and biophysical variables along climatic gradients and at ecologically relevant scales (i.e. relevant to the phenomena being investigated). It is evident from the literature that present monitoring programs and initiatives, remote sensing and non-remote sensing alike, are too scarce (far and few between) and too randomly scattered geographically (Walker & Raynolds, 2011).

Within the realm of the current remote sensing studies and the existing methodological and theoretical gaps, there exist ample opportunities to explore additional means and methods for retrieving quantitative estimates of vegetation biochemical and biophysical variables from untested sensors/platforms (Bratsch et al., 2016; Liu et al., 2017). In sparsely vegetated tundra environments, where broadband, broad-scale satellite imagery (and their associated empirical methods) often mask local ecological heterogeneity (Laidler et al., 2008), imaging spectroscopy satellite sensors and evolving image analysis techniques, such as machine learning regression algorithms (MLRAs) and physically based radiative transfer models (RTMs), may provide more

robust spectral characterization and retrieval of biophysical and biochemical variables than standard VIs, thus enhancing our current monitoring and modelling capabilities (Laidler et al., 2003; Stow et al., 2004; Buchhorn et al., 2013; Liu et al., 2017).

The literature review conducted for this research provides evidence that deriving quantitative estimates of vegetation biochemical and biophysical constituents to assess ecosystem composition, quality, and/or processes from spaceborne multi-angle imaging spectrometers is non-existent for Arctic ecosystems. It is apparent from the literature that different remote sensing spatial, temporal, radiometric and spectral resolutions need to be considered to study signals of change in Arctic ecosystems, especially when the current nadir-looking multispectral remote sensing sensors and associated methods show limitations (Stow et al., 2004; Buchhorn et al., 2013; Davidson et al., 2016; Bratsch et al., 2016; Liu et al., 2017). Since reflectance from a target depends on wavelength and is determined by the intrinsic surface properties such as the structural and optical properties of the surface (Chen et al., 2003; Chopping, 2008; Ollinger, 2011), it can be theorized that a greater understanding of variability of the radiation field over various vegetated landscapes (i.e. multi-angle remote sensing) will allow for an improved understanding of the independent variables contributing to reflectance, thus helping to guide modelling efforts directed towards vegetation assessments and variable retrievals.

Multi-angular remote sensing of surface reflectance anisotropy has largely been used to derive information about the structural properties of vegetation (Asner et al., 1998; Deering et al., 1999; Sandmeier & Deering, 1999; Diner et al., 1999, 2005). Of the multi-angular studies completed, the majority have been carried out in forested ecosystems to map the structural properties of vegetation, such as tree spatial density (Sabol et al., 2002; Wessels et al., 2004; Chopping et al., 2006, 2008, 2009), LAI (White et al., 2002; Pocewicz et al., 2007; Stagaskis et al., 2010; Sykioti

et al., 2011), tree height (Kimes et al., 2006; Heiskanen, 2006, Chopping et al., 2008, 2009), foliage clumping (Chen et al., 2005; Leblanc et al., 2005), and canopy heterogeneity (Widlowski et al., 2001; Pinty et al., 2002). On the other hand, multi-angular remote sensing studies directed towards retrieving pigment leaf and canopy biochemical variability appear to be less common (Verrelst et al., 2008; Stagaskis et al., 2010; Sykioti et al., 2011; Hilker et al., 2011; Hilker et al., 2017). The multi-angular spectroscopic remote sensing studies directed towards deriving both biochemical and biophysical variables from vegetation have been completed in a limited number of environments, such as forests (Verrelst et al., 2008; Omari et al., 2013; Hilker et al., 2017), shrub lands (Stagaskis et al., 2010; Sykioti et al., 2011), and agricultural landscapes (Delegido et al., 2008).

The Arctic remote sensing literature shows that very limited research has been conducted on reflectance anisotropy of Arctic vegetation, with no studies using multi-angle imaging spectroscopy data to retrieve biochemical and biophysical vegetation variables using either empirical or physical retrieval methods. Despite this, it has been stated that an increased understanding of directional reflectance is required to relieve doubt over the applicability of vegetation modelling approaches (Blackburn & Pitman, 1999; Laidler & Treitz, 2003). Vierling et al. (1997), using spectro-directional data collected *in situ*, showed larger VI differences exist in the forward scatter direction than in the backscatter direction and VI differences are significantly more pronounced at progressively larger solar zenith angles. These results suggest that there may be a need to account for the directional effects over the Arctic due to the extreme sun/sensor angles, given that non-nadir views typically provide different fractions of viewed shade/sunlit canopy and background (e.g. soil contributions). Multi-angular observations may be able to benefit our understanding of specific vegetation variables/characteristics in Arctic canopies in relation to their

spectro-directional effects thus increasing the potential for accurate retrievals from space. It is evident from the literature that there is a general lack of testing across environments using both empirical and physical techniques to estimate biochemical and biophysical constituents from multi-angular remote sensing data.

The CHRIS/PROBA satellite is one of the first spaceborne sensors to provide spectroscopic data at multiple viewing angles with a high spatial resolution. CHRIS images an area of approximately $14 \text{ km} \times 14 \text{ km}$, has a spatial ground resolution ranging from $\sim 34 \text{ m}$ to $\sim 17 \text{ m}$ (depending on viewing angle), and measures 62 spectral bands in the range of $\sim 411 \text{ nm}$ to 1050 nm with an average bandwidth of $\sim 10 \text{ nm}$. The CHRIS instrument is programmable so that a variety of band selections are possible. Most importantly, the agile pointing capability of the PROBA platform in both along track and across track directions gives CHRIS the ability to image all parts of the Earth's surface, well outside the instrument's nominal field of view of 1.3° (Fletcher, 2004). Images of a single site are generally acquired in sets of five at along track angles of: $\pm 55^\circ$, $\pm 36^\circ$, and 0° (nadir). The advantage of the CHRIS sensor is that it provides valuable spectral data for testing and validating the angular properties of reflectance models at the canopy scale. It is therefore of interest to investigate how spaceborne, spectro-directional data can contribute to monitoring biochemical variability in the Canadian Arctic.

2.2.2. Empirical modelling: Parametric and non-parametric regression

The estimation of vegetation variables from spectroscopic/remote sensing data is most commonly approached through empirical modelling methods (Darvishzadeh et al., 2008a; Zhao et al., 2013; Verrelst et al., 2015a,b; Verrelst et al., 2016). Empirical methods are used to find a statistical relationship between raw reflectance or a parameterized expression of reflectance and a measured variable of interest (e.g. LCC, PAI, CCC, etc.) (Kumar et al., 2006; Darvishzadeh et al.,

2008a; Croft et al., 2014; Verrelst et al., 2015a,b; Verrelst et al., 2016). Two common empirical modelling approaches include: (1) parametric linear regression based on VIs (i.e. univariate approaches) and (2) non-parametric non-linear MLRAs (i.e. multivariate approaches) (Verrelst et al., 2015a,b; Verrelst et al., 2016).

The use of linear parametric regression approaches for identifying the optimal narrowband VIs for quantifying the pigment biochemical and biophysical structural aspects of vegetation is a common approach and has been demonstrated in many studies (e.g. Stagaskis et al., 2010; Sykioti et al., 2011; Buchhorn et al., 2013; Verrelst et al., 2015a; Liu et al., 2017). Studies such as these have shown that narrowband VIs can be developed which have strong relationships to the variables of interest. However, it has been shown that methods based on linear parametric regression may not always be optimal when datasets are complex and exhibit non-linear attribute relationships, as is typical for spectroscopic data (Verrelst et al., 2015a,b; Verrelst et al., 2016). Although the practice of using two or more wavelengths to parametrize VIs is both conceptually and practically appealing, it is a reductionist approach (Zhao et al., 2013). In contrast to the linear parametric approaches, non-parametric non-linear MLRAs exploit the full reflectance signal (Verrelst et al., 2015a,b; Verrelst et al., 2016). Furthermore, non-parametric methods are often considered more useful in remote sensing studies since the data often have unknown distributions (Mountrakis et al., 2011). The variety of non-linear, non-parametric MLRA models has increased in recent years (e.g. random forests, support vector machines, artificial neural networks, kernel ridge regression, relevance vector machines, and Gaussian processes regression) (see Verrelst et al., 2015b; Verrelst et al., 2016). These methods apply non-linear transformation techniques and assume that no relationships exist between spectral features; therefore, the methodological advantage of non-linear non-parametric methods is their capability to model the non-linear relationships between

features without knowing their underlying data structures (Verrelst et al., 2015a,b). MLRAs have been shown to work well with a variety of data types such as highly dimensional spectroscopic data that exhibit a high degree of multi-collinearity (Verrelst et al., 2015a,b). Recent comparative studies have shown that Gaussian processes regression (GPR) is capable of outperforming other classes of MLRAs including linear parametric regression based on narrowband VIs for the retrieval of biophysical variables from airborne and satellite spectroscopic data (Verrelst et al., 2012c; Verrelst et al., 2015a; Verrelst et al., 2016).

Much of the present research using parametric and non-parametric empirical models to link vegetation biochemical and biophysical variables to imaging spectroscopy data has been conducted in agricultural landscapes (e.g. Haboudane et al., 2002; Colombo et al., 2003; Verrelst et al., 2015a), grasslands and shrublands (e.g. Darvishzadeh et al., 2008a; Stagaskis et al., 2010; Sykioti et al., 2011), and forests (e.g. Asner et al., 2008b; Huber et al., 2008; Verrelst et al., 2008). However, the retrieval of canopy variables from spectroscopic data in Arctic tundra ecosystems using either empirical approach has received much less attention in the literature (Liu et al., 2017). Although the use of narrowband VIs has been documented within Arctic ecosystems for estimation of canopy biophysical attributes (e.g. Buchhorn et al., 2013; Liu et al., 2017), there are currently no studies that have tested narrowband VIs for retrieving vegetation biochemistry (i.e. LCC and CCC) from spectroscopic data using either field or satellite based sensors. Further to this, there has not been a comparison of narrowband VIs to MLRA methods, specifically GPR, for retrieving biochemical (i.e. LCC and CCC) and biophysical variables (i.e. PAI) from field or spaceborne spectroscopic sensors.

2.2.2.1. Parametric regression: Vegetation indices - VIs (multi-band and pre-defined)

One of the most common retrieval methods used in optical remote sensing science and ecological monitoring programs is based on linear parametric regression using VIs (e.g. Darvishzadeh et al., 2008a; Croft et al., 2014; Verrelst et al., 2015a,b; Verrelst et al., 2016). Parametric regression methods relate spectral expressions (through either reflectance values or VIs) to a measured biophysical or biochemical variable of interest (e.g. LCC, PAI, CCC, etc.) (Croft et al., 2014; Verrelst et al., 2015a,b). VIs are mathematical transformations of reflectance designed to enhance spectral features sensitive to a biophysical or biochemical variable of interest while suppressing any unwanted reflectance background noise (Bannari et al., 1995; Wu et al., 2008; Glenn et al., 2008; Croft et al., 2014; Clevers et al., 2014; Garbulsky et al., 2011; Gitelson et al., 2006; Zhao et al., 2013). VIs are typically formulated to use wavelength regions with known sensitivities to specific vegetation properties (e.g. leaf pigment biochemicals, leaf non-pigment biochemicals, leaf internal structure or canopy structure) and are thus typically based on reflectance from wavelengths in the visible (~400 nm to 700 nm), red-edge (~690 nm to 720 nm), and near-infrared (NIR) (~720 nm to 1300 nm) (Filella & Penuelas, 1994; Filella et al., 2005; Gitelson et al., 2002b; Gitelson et al., 2003; Blackburn, 2007; Croft et al., 2014; Liu et al., 2017). Some VIs are designed to be sensitive to leaf and canopy water or lignin/cellulose content and generally include short-wavelength infrared (SWIR) wavelengths (~1050 nm to 2500 nm). As it was not possible to incorporate the SWIR region in the field and satellite spectral data and analysis of this research, such VIs are not considered further. The use of targeted spectral features (i.e. spectral regions) has been shown to reduce the effects caused by: (1) variations in unintended vegetation/leaf types or canopy properties, (2) soil/background reflectance, (3) sun and viewing geometry, and (4) atmospheric composition (Wu et al., 2008; Verrelst et al., 2015b).

There are numerous VI formulations found within the remote sensing literature that have been developed for retrieving plant based biochemical and biophysical variables (Blackburn, 2007). Extensive testing and comparisons of VIs have been previously conducted (e.g. Le Maire et al., 2004; Croft et al., 2014; Syskioti et al., 2011). Typical indices can be classified into four categories: (1) reflectance values at a single wavelength or in a wavelength range (hereafter referred to as “spectral band” or simply “band”) or a difference between reflectance in two spectral bands; (2) simple ratio of reflectance in two bands; (3) normalized difference ratios of reflectance in two bands; (4) indices based on reflectance signature derivatives (Verrelst et al., 2015a) such as spectra slope that are theorized to correct for the variation in leaf surface scattering and bidirectional reflectance effects and background reflectance (Vogelmann et al., 1993; Croft et al., 2014). The latter indices were not investigated in this study, as only the most commonly used VI formulations were selected.

It can be theorized that the widespread use of VIs is attributable to the simplicity of approach coupled with complete model transparency. VIs were first developed for use with broadband satellite sensors with very few spectral bands (Pearson & Miller, 1972; Bannari et al., 1995; Verrelst et al., 2015b). As spectroscopy in vegetation studies expanded from the lab and field to airborne and satellite imaging (Milton et al., 2009), particularly with the development of imaging spectrometers and increased computing power, the number of potential methods for information extraction also increased; optimized band information extraction algorithms based on previously designed band formulations were eventually developed for use with these large spectral datasets (Verrelst et al., 2015b). With the implementation of such algorithms it became possible to identify optimal bands for VI formulation by correlating all possible band combinations with the variable of interest (e.g. Darvishzadeh et al., 2008a; Darvishzadeh et al., 2011; Le Maire et al., 2008;

Mariotto et al., 2013; Rivera et al., 2014b; Verrelst et al., 2015a,b). However, the selection of the same optimal bands between studies for common biochemical and biophysical variables has not been reported in the literature (Verrelst et al., 2015a,b), indicating that such optimized VIs are often case/locally specific and lack generic capacity (Gonsamo, 2011; Heiskanen et al., 2013; Mariotto et al., 2013; Verrelst et al., 2015a).

Despite the lack of generalization of selected optimal bands in many VIs, the methodological approach can be generalized, for example using regression calibrated with ground data (i.e. the same technique/procedure is applied) to derive functions specific to the given environmental and site conditions (Verrelst et al., 2015b), sensor properties (band definitions, signal to noise, view angle, etc.), measurement scales, and sun-view angle geometry. This lack of generalizability can sometimes be partially mitigated through the optimization of the VI using large datasets that broadly encapsulate the expected systemic variability (Haboudane et al., 2004; Le Maire et al., 2004, Le Maire et al., 2008; Verrelst et al., 2015b). However, it must be noted that use of just a few spectral bands transformed to a VI cannot be expected to fully capture the complexity of the real world, especially across varied and diverse environments.

The basic principle behind parametric regression using VIs entails mathematically defined combinations of spectral bands regressed against a variable using a fitting function, where fitting functions can be either linear or non-linear (e.g. curve fitted to a series of data points) (Cohen et al., 2003; Verrelst et al., 2015a,b). In general, this VI approach, when used in a spectroscopic framework, is challenging and presents methodological problems since there are a variety of choices that must be made in the modelling process. Such choices/problems include: (1) the selection of optimal bands/wavelengths (often complicated by variable covariation), (2) selecting the best VI formulation (there are numerous index transformations), and (3) determining the

optimal calibration fitting function (e.g. linear vs. polynomial). These factors have the ability to positively or negatively influence the outcome of the model estimation/prediction (Rivera et al., 2014b; Verrelst et al., 2015b).

Preceding the selection of the preferred VI, there is often a need for systematic assessment of spectral band combinations in a given VI formulation since formulations are not universal (Verrelst et al., 2015a,b). For example, the common Normalized Difference Vegetation Index (NDVI, Equation 1) (Rouse et al., 1973) can be assessed using all possible two-band combinations:

$$NDVI_{a,b} = (\rho_b - \rho_a) / (\rho_b + \rho_a) \quad (1)$$

where $\rho_{a,b}$ is the reflectance in bands a and b within the entire spectral range being considered. Such assessment permits the selection of the best performing wavelengths for the given VI formulation based on correlation analysis with reference data for the given vegetation variable (Verrelst et al., 2015a,b).

All VI formulations have the ability of being evaluated using all available sensor bands, however, most rely on the use of two band formulations (Bannari et al., 1995; Verrelst et al., 2015b). In the visible near-infrared (VNIR), these predefined/published VIs are typically comprised of a reference wavelength between 750-900 nm where reflectance responds to vegetation structure and a wavelength between 650-720 nm where leaf pigments absorb most irradiance (Sims & Gamon, 2002; Croft et al., 2014). A potential problem of two-band VIs is that they can give saturated values for the biochemical or biophysical variable in question, particularly where woody vegetation is present (e.g. NDVI values reach an asymptote at high LAI values – adding more leaves to a canopy will not increase the NDVI values). It has been shown that this problem can partially be overcome by optimizing the band selections (Delegido et al., 2011; Delegido et al., 2013; Verrelst et al., 2015a,b). Alternatively, three-band spectral VIs have been

proposed to avoid this saturation problem (Wu et al., 2008; Wang et al., 2012). However, increasing the number of bands in a VI can substantially increase the possible number of band combinations, especially when dealing with spectroscopic datasets with many bands. For example, if using a spectroradiometer with 750 channels and using a VI with three possible wavelengths, the total number of permutations will be ~420 million and the total number of combinations will be in the order of ~70 million. There are numerous published VIs in the remote sensing literature that have been tested (e.g. Le Maire et al., 2004; Croft et al., 2014; Syskioti et al., 2011). The common multi-band VIs that were used in this research project can be found in Chapter 5, Table 24. To complete this research in a timely manner, only two-band VIs were used for the multi-band component of the VI modelling.

As an alternative to investigating all band combinations through a VI formulation, there are many published narrowband VIs that have been developed (i.e. optimized) for estimation of leaf pigment content (e.g. LCC) and canopy structural variables (e.g. PAI), using some combination of one, two or three bands through the four common formulations listed above (Le Maire et al., 2004; Blackburn et al., 2007; Ustin et al., 2004; Croft et al., 2014). The benefits of using predefined/optimized VIs are that: (1) they have been previously investigated for their efficacy using specific wavelengths, and (2) there is no need to systematically explore all band combinations as described above. However, in most cases these VIs have been tested for only one or at most a few related species (usually at the leaf scale) for specific environments and thus it is not clear whether they can be applied across species with varying leaf structural characteristics or in not previously tested environments with varying canopy structures and soil backgrounds (Sims and Gamon, 2002; Ustin et al., 2009; Zhao et al., 2013; Croft et al., 2014).

An example of such a published VI is the greenness vegetation index (GVI) (Equation 2), which was formulated specifically to exploit plant greenness/chlorophyll content (Gandia et al., 2004):

$$GVI_{553,682} = (\rho_{682} - \rho_{553})/(\rho_{682} + \rho_{553}) \quad (2)$$

The detection of individual pigments (e.g. chlorophylls) has been given less attention by the remote sensing community than total pigment measures, despite the importance of pigments for parameterizing physical modelling or for ecological monitoring (Blackburn 2007; Ustin et al., 2009). This is due to the difficulty in resolving the overlapping absorption regions of individual pigments and their high degree of autocorrelation (Chappelle et al., 1992; Ramsey & Rangoonwala, 1995; Blackburn, 1998a,b, Grossman et al., 1996). Since pigments have distinctive absorption spectra depending on their molecular structure and local chemical environment (Ustin et al., 2009), the challenge is to properly account for the multiple factors influencing the retrieved signal, a task that could be addressed when using multiple wavelength combinations in a general VI formulation (e.g. VIs with one vs. two vs. three or more bands) (Ustin et al., 2009). Overall, the formulation of a VI should lead to optimal sensitivity with the vegetation variable of interest; however, there are many VIs, so the choice of optimal formulation is a difficult question, especially when there are overlapping absorption features of the desired variables (Ustin et al., 2009).

Once a formulation is selected, the calculated VI is correlated to field data of the variable of interest (e.g. LCC, PAI, CCC) using a fitting function, which expresses the relationship between the VI and the variable (Verrelst et al., 2015a). There are a variety of fitting functions that can be selected for calibration and validation, such as linear, exponential, logarithmic, polynomial, etc.). The process typically involves least squares fitting (i.e. the optimal VI is that which minimizes the sum of the squared errors in the fitted equation) (Verrelst et al., 2015a). The impact of the type of fitting function has been evaluated and shown to be small with respect to the impact of VI band

selection (Rivera et al., 2014b). It has also been shown that a linear function is usually sufficient where vegetation is sparse and does not saturate the VI signal (Darvishzadeh et al., 2008a; Verrelst et al., 2015a); therefore, a linear function was used in this research. Use of regression functions to derive optimal VIs has been criticized since there is a lack of uncertainty estimates for the outputs (Verrelst et al., 2015b). This point can lead to the conclusion, by some, that parametric regression methods are inadequate for operational extraction of vegetation biochemical and biophysical variables (e.g. Verrelst et al., 2015a,b).

2.2.2.1.1. Implementation of parametric regression based on VIs

The objective of employing linear parametric modelling in this research was to determine: (1) optimal spectral band configurations for selected predefined VIs, and (2) the usefulness of optimized narrowband VIs in predicting biochemical (leaf chlorophyll content, canopy chlorophyll content) and biophysical (LAI) variables using multi-angle spectroscopic data at the field and remote sensing scales in the Western Canadian Arctic. VIs that were selected for study included common ones such as NDVI, and narrowband VIs that have been successfully used for predicting vegetation biochemical and biophysical attributes in various environments. Formulations selected were also based upon their ability to reduce unwanted background effects, such as soils (e.g. SAVI) (e.g. Wu et al., 2008). It is possible that VIs that account for such factors as soil reflectance may be able to better predict biochemicals at the canopy scale than those that do not, particularly for low density Arctic vegetation where canopy gaps are common. Standard VIs, such as NDVI, are often preferred over soil based VIs in remote sensing since soil-based VIs require additional information on soil spectra and are computationally more demanding (Broge & Mortensen, 2002; Darvishzadeh et al., 2008a). Nevertheless, indices that account for background and structural reflectance contributions have been shown to overcome the limitations of standard VIs at the

canopy level (Haboudane et al., 2002). An attempt was made in this research to strategically explore many of the VIs currently used in remote sensing studies for estimating biochemical and biophysical variables (i.e. those based on plant greenness/leaf pigments). Table 24 in Chapter 5 shows a complete list of the VIs that were used. Figure 12 shows the modelling approach used at both the field and remote sensing scales. A sub goal of the investigation was to find the optimal VI for use across the Arctic, resistant to the effects of look/sun angle, spatial scale and spectral resolution, and to compare this method to machine learning and physically-based inversion.

Figure 12 Empirical modelling procedure based on parametric linear regression and VIs. All multi-angle spectral measurements were iteratively evaluated with the various VIs. All possible band combinations were evaluated with each VI and then compared against the biochemical and biophysical field measurements using linear regression. Modelling outcomes were evaluated and compared using the coefficient of determination (r^2) and error metrics, such as the root mean square error (RMSE).

2.2.2.2. Non-Parametric regression: Machine learning regression algorithms - MLRAs

A large methodological challenge imposed by spectroradiometry and imaging spectroscopy is that data are typically composed of highly correlated spectral bands (Weiwei et al., 2013; Verrelst et al., 2016). Consequently, the reduction of spectral dataset dimensionality is an important procedure that can improve modelling results, shorten model training times, reduce the potential of over fitting, and enhance the generalizability of the model (Curran, 1989; Grossmena et al.,

1996; Nansen et al., 2013; Verrelst et al., 2016). Variable reduction or feature selection can be accomplished either through automated techniques (e.g. Arenas-Garcia et al., 2013; Verrelst et al., 2016) or by selecting spectral bands that best highlight the biophysical variable in question. Manual band selection is commonly based on expert knowledge of the variable of interest that can suppress responses from unwanted variables/features (Darvishzadeh et al., 2008a), however, it may not always be applicable when applied to new ecosystems or plant species or when unknown predictive variable relationships exist. Algorithmic spectral band selection and variable reduction can therefore be viewed as an optimization approach where the intended goal is to select a subgroup of spectral variables/features that captures the most predictive information and accordingly best explains the predicted variable (Verrelst et al., 2016).

Within the context of machine learning, feature selection (or variable reduction) is the process of selecting the most important subset of predictor variables to be used in the construction of the predictive model. Feature selection methodologies/algorithms can be categorized into two basic groups: (1) filter methods (Liu & Motoda, 1998) and (2) wrapper methods (Kohavi & John, 1997; Verrelst et al., 2016). (1) *Filter methods* select a subset of features independent of the algorithm (no interaction with the algorithm) (Verrelst et al., 2016). These model types are typically based on statistical correlation of the selected features with the predicted variable; the least useful/redundant features are suppressed while the selected features are chosen to be a part of the final regression/predictive model. An example of the filter method is the systematic calculation of all possible band combinations through a generic VI, the resulting VI values being regressed against the vegetation variable of interest, and the performance of each model evaluated based on a score/measure such as the determination coefficient, r^2 (Rivera et al., 2014b; Verrelst et al., 2015a; Verrelst et al., 2016). Filter methods commonly exhibit faster convergence times (i.e.

model completion time) than wrapper methods since they are computationally less demanding (Verrelst et al., 2016); however, as previously noted, such VI optimization processes are limited to three or fewer variables to avoid computational overloading. (2) *Wrapper methods*, on the other hand, evaluate all possible subsets of features of the dataset, which in turn allows the detection of possible interactions between features (i.e. they are full-spectrum and evaluate all band combinations in the dataset, not just feature structures based on pre-defined VI band possibilities) (Verrelst et al., 2016). Wrapper methods use the regression output as the criteria for model selection, an approach that allows for model improvement with each algorithmic step (Verrelst et al., 2016). Disadvantages of wrapper methods are that they are complex and difficult to implement, they require parameter tuning, and they can be computationally demanding. Disadvantages of both types of machine learning methods described above are: there is an increased overfitting risk when the number of observations is insufficient, and the computation time can become significant when the number of variables is large, such as in the case of full spectrum data (thus the requirement to reduce dimensionality) (Verrelst et al., 2015b). However, procedures such as cross-validation may help to reduce overfitting problems in machine learning (Cawley & Talbot, 2010).

Both filter and wrapper methods have been used for the identification of spectral bands as they relate to vegetation properties; however, much of this work has been for classification purposes (e.g. Pal & Foody, 2010; Moutrakis et al., 2011). There are very few studies concerned with the retrieval and estimation of vegetation properties (e.g. leaf biochemical content) with wrapper methods. Verrelst et al. (2015b) compared the use of filter vs. wrapper methods for the estimation of vegetation properties (i.e. leaf and canopy chlorophyll, LAI) using spectroscopic data. They then investigated the use of a wrapper method, GPR, for the estimation of LAI using hyperspectral remote sensing data (Verrelst et al., 2016). Both studies showed high levels of success compared

to the other retrieval methods (e.g. Verrelst et al., 2015b; Verrelst et al., 2016). Considering the above, the focus of this research was on the use of wrapper methods.

Optimization in machine learning regression methods is implemented using training data in a learning stage. Assumptions about the structure of the training data can either simplify or complicate the algorithm training process and thus affect model outcomes (Verrelst et al., 2016). Parametric methods assume an underlying structure of the training data distribution whereas non-parametric methods do not. Non-parametric methods are slower to train as they require more training data and are more complex, but they have been shown to produce better predictions (Verrelst et al., 2015a). Furthermore, non-parametric methods are often considered more useful in remote sensing studies since the data often have unknown distributions (Mountrakis et al., 2011). They can be further subdivided into linear and nonlinear models. Linear non-parametric regression models may be chosen because they offer good predictive performance and the algorithm is generally more simplistic than non-linear non-parametric methods; however, they may not be suitable with complex datasets that exhibit non-linear attribute relationships, as is typical for spectroscopic data (Verrelst et al., 2015a,b). Linear regression methods characteristically depend upon the estimation of covariance (i.e. the joint variability between two random variables), which can be problematic when severe multi-collinearity increases the variance of the coefficient estimates, thus making the estimates extremely sensitive to minor model changes (i.e. the coefficient estimates are unstable and difficult to interpret). As noted before, to reduce multi-collinearity, linear methods are usually accompanied by some form of dimensionality reduction (Verrelst et al., 2015a,b). There are a handful of linear parametric approaches which have been used in remote sensing, including stepwise multiple linear regression (SMLR), principal component regression, partial least squares regression (PLSR), ridge regression, and least absolute shrinkage and selection

operator (Verrelst et al., 2015b). SMLR (Dorigo et al., 2007; Verrelst et al., 2015a) and PLSR (see Verrelst et al., 2015b) are widely applied for the selection of spectral bands related to vegetation biochemical and biophysical attributes. Darvishzadeh et al. (2008a, 2011) found that PLSR produced better results than SMLR in a heterogeneous grassland environment. Linear methods are increasingly being replaced by non-linear non-parametric algorithms since they have been shown to produce better results and are therefore better able to handle large multi-dimensional spectroscopic datasets (Verrelst et al., 2015a,b). Hence, the intention in this research was to focus on the use of wrapper-based non-linear, non-parametric MLRA.

Non-linear, non-parametric MLRAs can be separated into three distinct groups (1) decision tree learning, (2) artificial neural networks (ANNs), and (3) kernel methods. Decision trees and ANNs have been well described in the literature (see Verrelst et al., 2015b); therefore, only their applicability in remote sensing is briefly summarized here.

Not until recently have decision trees gained traction in the remote sensing literature (e.g. Hansen et al., 2002; Im et al., 2009, Im et al., 2012; Viedma et al., 2012). Most of these studies have used algorithms such as bagging trees and random forests, for classification purposes instead of regression applications (i.e. prediction of geo-physical variables). Random forest regression appears to have gained the most traction in modelling and prediction of vegetation attributes such as biomass (Adam et al., 2014; Vaglio Laurin et al., 2014), canopy cover (Gessner et al., 2013), leaf area (Vuolo et al., 2013), and canopy nitrogen (Li et al., 2014a), generally outperforming conventional parametric and linear non-parametric methods (Verrelst et al., 2015b).

ANNs have been used extensively for mapping vegetation properties with remote sensing data (Jin & Liu, 1997; Paruelo et al., 1997; Franci & Panigrahi, 1997; Kimes et al., 1999; Kavzoglu & Mather, 2003). The advantage of ANNs compared to linear models based on VIs has been

demonstrated (Verrelst et al., 2015b). More recent applications include the estimation of foliar nitrogen concentrations (Huang et al., 2004) and LAI (Jensen et al., 2012) from spectroscopic data. Both studies demonstrated higher accuracies as compared to linear non-parametric models, such as PLSR. More complex recurrent ANNs and radial basis function ANNs have recently been used to map vegetation properties (Chai et al., 2012; Li et al., 2013; Wang et al., 2013). Because of the complexity of ANNs there has been motivation to use simpler MLRAs (Verrelst et al., 2015b). When compared to kernel based MLRAs (described below), ANNs can be unstable, producing a wide range of modelling outcomes (Verrelst et al., 2012a,b; Verrelst et al., 2015b).

Kernel methods use a similarity function that measures the similarity between data points; they are also known as a covariance functions) (Shawe-Taylor & Cristianini, 2004; Verrelst et al., 2015b). In machine learning, they quantify the similarities between input samples of a calibration dataset. Kernel methods essentially transform a dataset's feature space into a higher dimensional feature space that then allows for the machine learning algorithm to more easily determine the differences between data points (e.g. when moving from two dimensional to three-dimensional space, the differences/separability between points are more easily determined). Kernel methods have been used for the past decade in remote sensing, particularly with support vector machines (SVM) used for classification purposes (Mountrakis et al., 2011), but also for vegetation biochemical and biophysical variable estimation (Karimi et al., 2008; Yang et al., 2011; Verrelst et al., 2015b, Verrelst et al., 2016), such as support vector regression (SVR) (Vapnik et al., 1997), relevance vector machines (RVM), kernel ridge regression (KRR), and GPR (Rasmussen & Williams, 2006).

Comparative studies have shown that not all MLRAs such as those described above perform to the same standard, but in general they do outperform linear non-parametric methods (e.g. Verrelst

et al., 2015a,b; Yang et al., 2012; Yang et al., 2011; Karimi et al., 2008; Wang et al., 2011). Verrelst et al. (2015b, 2016) have shown that GPR was capable of outperforming other MLRAs for the retrieval of biophysical variables from airborne and satellite spectroscopic images. Verrelst et al. (2015b) compared GPR with parametric methods based on established and generic VIs; GPR outperformed VIs and other MLRAs, but also offered additional features, such as an indication of spectral band relevance, the weight of the most relevant spectra contained in the dataset, and probabilistic outputs (e.g. mean estimate and associated uncertainty). Verrelst et al. (2016) investigated GPR in combination with a band analysis tool (BAT) for spectral analysis of vegetation properties (Camps-Valls et al., 2016). Although GPR has been used in these experimental studies, it has not been fully tested across environments and spectroscopic sensors (Verrelst et al., 2015a; Verrelst et al., 2016). Furthermore, the GPR-BAT has also not been tested across environments and sensor types or in an operational sense. This research provided an opportunity to evaluate it further in Arctic hyperspectral satellite vegetation modelling. The following summarizes the GPR algorithm and its implementation within this research.

2.2.2.2.1. Gaussian Processes Regression (GPR)

Within the context of machine learning, the approximation of the optimal regression function for variable prediction is a common question; this issue can be reduced to finding the best predictor function from a group of possible functions (Verrelst et al., 2016). The optimal function can typically be found/learned through the simultaneous minimization of a defined cost function accounting for prediction error and through some predefined regularization term that controls/constrains the cost function's capacity (Du & Swamy, 2014; Verrelst et al., 2016). Further to this, the identification of the optimal regression function can be approached within a Bayesian non-parametric framework; GPR operates within this context (Rasmussen & Williams, 2006;

Camps-Valls et al., 2016; Verrelst et al., 2016). GPR is a kernel based non-parametric probabilistic method that provides a full statistical description of the predicted variables that can be used to interpret confidence intervals and to set/test kernel parameters/hyperparameters (Verrelst et al., 2016).

A Gaussian process is a collection of random functions, any finite number of which have consistent joint Gaussian distributions (Rasmussen & Williams, 2006). Simply put, a Bayesian linear regression approach provides a probabilistic approach to finding model parameters whenever new data points are observed, whereas a GPR approach assumes that an *a priori* Gaussian process governs the set of all possible unobserved latent functions that are consistent with the observed/known data (Rasmussen & Williams, 2006; Verrelst et al., 2016). The likelihood of the latent functions combined with the known data observations allows for posterior probabilistic estimates of the predicted variable (Verrelst et al., 2016). A full description of the GPR algorithm is provided elsewhere (e.g. Rasmussen & Williams, 2006; Verrelst et al., 2016).

All kernel methods, including the GPR algorithm, use a kernel or covariance function (k). A standard and commonly used covariance function is the squared exponential (Equation 3):

$$k(x_i, x_j) = \exp\left(-\frac{\|x_i - x_j\|^2}{2l^2}\right) \quad (3)$$

where x_i, x_j is the distance between two points and l is the length scale (i.e. a term that describes how smooth the function is). This covariance function captures sample similarities well in many problems and only has one model hyperparameter that requires tuning (l); however, kernels with more hyperparameters can also be efficiently implemented within the Gaussian processes framework (Verrelst et al., 2016). A GPR modelling approach made available by Verrelst et al. (2016) provides the implementation of the anisotropic squared exponential kernel function, which

allows for the exploitation of asymmetries in the feature space by including hyperparameters for each input feature. The anisotropic squared exponential covariance function (Equation 4) can be written as:

$$k(x_i, x_j) = \sigma^2 \exp\left(-\sum_{b=1}^B \frac{(x_i^b - x_j^b)^2}{2l_b^2}\right) + \sigma_n^2 \delta_{ij} \quad (4)$$

where model hyperparameter σ^2 is a scaling factor (i.e. signal variance, which determines variation of function values from their mean), σ_n is the standard deviation of the estimated noise (i.e. noise variance, not typically a part of the covariance function but used by Gaussian processes to allow for noise present in the training data), l_b is the length-scale for each input feature (i.e. spectral band) $b = 1, \dots, B$, and δ_{ij} is the difference between i and j (the noise variance is only applied when $i = j$) (Verrelst et al., 2016). The model hyperparameters (σ^2 , σ_n , l_b) and model weights (α_i) are automatically optimized during the modelling/training process, where the obtained weights after optimization provide the relevance of each spectrum x_i and inverted values of l_b indicate the relevance of each spectral band (Verrelst et al., 2016). Lower l_b values provide an indication of a higher predictive power of a band to the training function (k) (Verrelst et al., 2016).

This modified GPR model of Verrelst et al. (2016), which uses the squared exponential covariance/kernel function, provides a wrapper based algorithm that operates in a backwards approach; the impact of the input features on the prediction error is assessed in the presence or absence of the other features. At each algorithmic step, the model kicks out the least significant spectral bands with the highest l_b values and retrain a new model with those features (bands) which remain (Verrelst et al., 2016). This sequential backward band removal (SBBR) operates in the same way as recursive feature elimination (RFE), which is applied in SVM classification (Mountrakis et al., 2011). RFE works by removing the features with the smallest ranking scores to

recursively eliminate insignificant features (Pal & Foody, 2010; Mountrakis et al., 2011). The goal of using the SBBR algorithm is to move backwards until only one band is left as the most related to the biochemical or biophysical variable under investigation. Specifically, the SBBR algorithm works as follows. For a given number of bands in the spectral dataset: (1) split the spectra/variable dataset into training-validation groups; (2) train the GPR model; (3) rank each spectral band using a metric determined by the model hyperparameter (l_b); (4) calculate score metrics in the validation of the model (e.g. coefficient of determination, r^2 and root mean square error, RMSE); (5) remove the spectral bands with the highest l_b values; (6) repeat until all bands are tested (Verrelst et al., 2016).

Verrelst et al. (2012a,b) demonstrated the usefulness of SBBR for identifying the most relevant spectral channels when retrieving vegetation variables from spectroscopic data, and furthermore, accurate retrieval was achieved using a minimal number of spectral bands. It was also shown in Verrelst et al. (2012b; 2015b; 2016) that this method can achieve higher accuracies than parametric filter-based vegetation index methods that systematically analyzed all two band combinations with the NDVI formulation and the optimal bands were shown to possess physical meaning with respect to the variables in question (Verrelst et al., 2012b, Verrelst et al., 2015a,b; Verrelst et al., 2016).

2.2.2.2.2. GPR – Band Analysis Tool (GPR-BAT) and implementation

The SBBR routine described above has been implemented in the ARTMO (Automated Radiative Transfer Models Operator) software within the MLRA toolbox as the Gaussian Processes Regression Band Analysis Tool (GPR-BAT) (Rivera et al., 2014a,b; Verrelst et al., 2016). It was adopted for this research.

The GPR-BAT algorithm, like the SBBR, allows for the evaluation of the predictive power and ranking for each band for the variable of interest through the calculation of the kernel/covariance function hyperparameters (Rivera et al., 2014a,b; Verrelst et al., 2016). It is capable of being combined with the k -fold cross validation technique; cross-validated results are typically averaged in the final outputs to produce a more robust validation estimate (Verrelst et al., 2015a,b).

The objectives of testing the GPR-BAT algorithm in this research were to: (1) identify how many spectral variables (bands) are minimally needed to produce robust results, and of those, which are the most important/sensitive wavelengths for predicting the variable in question, and (2) determine the usefulness of GPR in prediction of biochemical (leaf chlorophyll content, canopy chlorophyll content) and biophysical (LAI) variables using multi-angle spectroscopic data at the field and remote sensing scales in the Western Canadian Arctic. (Verrelst et al., 2016). The GPR-BAT routine summarized in the Figure 13 below shows the implementation within this research project.

Figure 13 Empirical modelling based on the non-parametric multi-variate GPR-BAT algorithm. All multi-angle spectral measurements were iteratively evaluated with the GPR algorithm. For each set of multi-angle spectra, all band combinations were evaluated for predicting the biochemical and biophysical field measurements. With each model iteration the least contributing spectral band was removed until the optimal predictive band(s) remained. Predictive performance of the optimal band(s) was evaluated using r^2 and associated error metrics (e.g. RMSE).

2.2.3. Physical modelling: Radiative transfer models (RTMs)

Aside from the empirically based models, the estimation and retrieval of vegetation biochemical and biophysical variables from spectroscopic remote sensing data can also be approached through a physical modelling framework. RTMs, a commonly used physical modelling approach used in remote sensing, describe the transfer or interaction of radiation (i.e. absorption and scattering) with canopies (i.e. leaves, canopies, and soil) based on physical laws and therefore provide a generalizable and explicit link between the biochemical and structural characteristics of vegetation and top-of-canopy spectral reflectance (Jacquemoud & Baret, 1990; Verhoef, 1984; Houborg et al., 2007; Soenen et al., 2009; Darvishzadeh et al., 2008a; Jacquemoud et al., 2009). RTMs (of various configurations/physical treatments) have been extensively tested for their ability to simulate radiative transfer in a variety of naturally occurring environments, and as such are well documented within the remote sensing literature (e.g. Jacquemoud et al., 2009; Widlowsky et al., 2013). A comprehensive assessment of the physical realism of RTMs is provided by the continuing RTM Inter-comparison (RAMI) project (Pinty et al., 2001; Pinty et al., 2004; Widlowsky et al., 2007; Widlowsky et al., 2013). The PROSAIL RTM has become one of the most widely used leaf-canopy models due to its ease of use, robustness, consistent validation by lab/field/remote sensing experiments, code/model availability, and general importance within the remote sensing literature (Baret et al., 1992; Jacquemoud et al., 2009). PROSAIL is made up of the PROSPECT leaf model (Jacquemoud & Baret, 1990; Feret et al., 2008) and the SAIL canopy model (Scattering by Arbitrary Inclined Leaves) (Verhoef, 1984; Verhoef, 1985; Jacquemoud et al., 2009) and thus provides a means of simulating the spectro-directional reflectance of canopies.

At the leaf-level, the PROSPECT model is used to describe and simulate the directional-hemispherical reflectance of green and senescent monocotyledon and dicotyledon species in the

visible, NIR, and SWIR regions of the electromagnetic spectrum (i.e. 400 nm to 2500 nm). PROSPECT, which is based upon the plate model (Allen et al., 1969), describes the isotropic scattering and absorption properties of leaves as a function of two classes of input parameters: (1) the leaf structure parameter (scattering), which describes the air/cell wall interfaces within the mesophyll, and (2) the leaf biochemical content (absorption), which describes the quantity of pigment and non-pigment chemicals contained within the leaf structures (Jacquemoud et al., 2009). Since its introduction in 1990, PROSPECT has been updated to account for the following: (1) Bousquet et al. (2005) were able to add a physical description of directional reflectance properties of leaves, (2) Feret et al. (2008) were successful in separating the optical/absorption contributions of both chlorophyll and carotenoid pigments (i.e. PROSPECT-5), and (3) Feret et al. (2017) further improved PROSPECT-5 with the inclusion of anthocyanins (PROSPECT-D).

At the canopy level, the SAIL model, which is an extension of the one-dimensional model developed by Suits (1972), is used to simulate the bidirectional reflectance factor (BRF) (Schaeppman-Strub et al., 2006) of turbid medium plant canopies (Jacquemoud et al., 2009). The SAIL model provides top of canopy BRF simulations by solving the absorption and scattering of four-stream (upward/downward) radiative fluxes (Verhoef, 1985; Jacquemoud et al., 2009). The original SAIL formalism has also given rise to several different versions (see Jacquemoud et al., 2009). For example, SAILH is a turbid medium model that has been fitted with a hotspot parameter (a function of the ratio of leaf size to canopy height) that idealizes the canopy to be spatially homogenous (Kuusk, 1991). SAILH describes canopy BRF as a function of the following classes of input parameters: (1) canopy structure (e.g. leaf area, leaf angle), (2) background reflectance (e.g. soil reflectance), (3) radiation behaviors and observation parameters (e.g. hot-spot, diffuse/direct radiation, sun/sensor geometry). In general, canopy models range from one-

dimensional models (e.g. SAILH), where the vegetation canopy is presumed to be a turbid medium with randomly distributed elements, to three-dimensional models (e.g. Li & Strahler, 1992), where the canopy is presumed to be horizontally heterogeneous or discontinuous. While three-dimensional models are applicable to horizontally heterogeneous or discontinuous canopies (such as isolated tree crowns), one-dimensional RTMs (e.g. PROSAIL) have been used for canopies such as heterogeneous grasslands (Darvishzadeh et al., 2008a,b). Given the nature of Arctic tundra canopies, which consist of mostly low-lying, spatial uniform vegetation configurations when observed at the remote sensing scale, a 1D model should theoretically be ideally suited for simulating top-of-canopy spectro-directional reflectance.

Significant efforts to retrieve vegetation biochemical and biophysical properties from RTMs have been carried out in a multitude of environments. These studies include: (1) agricultural crops (Jacquemoud et al., 1995; Weiss et al., 2001; Kempeneers et al., 2008; Verger et al., 2011; Duan et al., 2014; Verrelst et al., 2015a), (2) grasslands (Darvishzadeh et al., 2008a,b; Darvishzadeh et al., 2011; Atzberger et al., 2015), and (3) forests (Zarco-Tejada, 2004; Undelhoven et al., 2000; Peterson, 1988; Fourty et al., 1996; Feret & Asner, 2011; Hilker et al., 2017). A review of the remote sensing literature reveals that there are no studies that have investigated the use RTMs (i.e. PROSAIL) and their inversion for retrieving biochemical (i.e. LCC and CCC) or biophysical (i.e. PAI) variables from imaging spectroscopy data (neither field nor spaceborne) in Arctic tundra environments. This is a novel component to this research project.

2.2.3.1. Physical modelling: Inversion of leaf and canopy RTMs

To make leaf and canopy RTMs useable for parameter/variable retrieval, they need to be inverted (Darvishzadeh et al., 2008a,b; Jacquemoud et al., 2009; Verrelst et al., 2015a,b). Inversion with remote sensing spectra/data can be treated as a physically meaningful method for retrieving

leaf and canopy biochemical and biophysical variables since the physical laws incorporated into RTMs are considered universal and therefore theoretically applicable across ecosystems – should the model be complex enough to account for the biochemical and biophysical complexities of the intended system (Dorigo et al., 2007; Verrelst et al., 2015a,b). Despite their conceptual simplicity, physical models and associated inversion techniques are not straightforward due to the inherent complexity of the RTM (i.e. several parameters are generally required to describe the system) and the multiple choices and implementation issues involved with running the model in reverse. Foremost in advance of any retrieval attempt, a RTM model must be selected whereby a trade-off between realism and inversion feasibility is made (Verrelst et al., 2015a,b). Complex models will typically provide a better description of the physical system in which they are being implemented but they are difficult to invert since they possess many variables. It may also be difficult to provide physical measurements for every parameter in the model. On the other hand, simple RTMs may not account for the complexities inherent in the physical system, however, they are easier to invert since there are few variables describing the system (Verrelst et al., 2015a,b). One of the major considerations that must be made for physical model inversion concerns the Hadamard postulates (Hadamard, 1902), which state that RTMs are only invertible under the following conditions: (1) a solution exists, (2) the solution is unique, and (3) the solution's behavior changes continuously with the initial/starting conditions (Hadamard, 1902; Verrelst et al., 2015b). In mathematical terms, when a problem meets these conditions it is considered well-posed. However, these conditions are seldom met in remote sensing; the inversion of RTMs is mostly under-determined and ill-posed since the radiometric signal carries only limited information (Combal et al., 2002; Combal et al., 2003; Baret & Buis, 2008; Jacquemoud et al., 2009). Furthermore, and probably the biggest problem, is that various combinations of input parameters (spectral band reflectance) typically

result in the same solution (i.e., the same biophysical or biochemical attribute values). These major disadvantages, specifically within a remote sensing framework, make physically-based retrievals of vegetation biochemical and biophysical variables a challenging task and thus present the principal hindrance towards operational use.

The inversion of RTMs is typically completed using one of three methods: (1) look-up-table (LUT) inversion, (2) iterative numerical optimization techniques, or (3) hybrid approaches (e.g. artificial neural networks) not discussed here (see Verrelst et al., 2015b). With each technique, there are ways to mitigate the ill-posedness of the problem. All methods have produced accurate results; however, there is a paucity of comparative studies (e.g. Vohland et al., 2010; Preidl and Doktor, 2011).

The LUT approach is considered by many to be the simplest and quickest method of inverting RTMs, and is likely the most widely used for inverting leaf and canopy RTMs (Dorigo et al., 2007; Darvishzadeh et al., 2008a,b; Darvishzadeh et al., 2012; Verrelst et al., 2015a,b). It works as follows. A large array of canopy reflectance values is generated in advance of the inversion through forward calculations using the given RTM code. All possible parameter combinations of the model variables (i.e. biochemical and biophysical values), usually constrained to measured or known values expected to occur, are used to shape the dimensionality of the LUT. To invert the model, the user simply identifies the parameter combinations that yield the best fit between measured and modelled results using a cost/merit function (Liang, 2007). Essentially, the cost function minimizes the summed differences between the simulated and measured reflectance for all wavelengths (Jacquemoud et al., 2009); RMSE is often used as the merit/cost function. To achieve a high accuracy for the estimated parameters, the dimensionality of the LUT must be sufficiently large and thus presents a formidable challenge to provide the correct model parameter ranges (Combal

et al., 2002; Combal et al., 2003; Tang et al., 2007; Weiss et al., 2000; Verrelst et al., 2015a,b). Dimensionality of the LUT can be reduced using expected or experimental parameter probability distributions (e.g. uniform or Gaussian) (Darvishzadeh et al., 2012).

Arguably, the main advantage of using LUT-based inversion is computational speed (Dorigo et al., 2007; Verrelst et al., 2015a,b). It only requires the generation of one spectral-vegetation attribute database, albeit with sufficient dimensionality, from which the vegetation attribute values corresponding to the measured spectra are extracted. There are various regularization procedures that can be adopted to optimize LUT and other types of model inversions. (1) The use of known parameter ranges can be used to constrain the dimensionality of the LUT (Combal et al., 2002; Darvishzadeh, et al., 2008a; Baret & Buis, 2008; Dorigo et al., 2009; Verrelst et al., 2012c; Verrelst et al., 2015b). For example, if leaf chlorophyll values are measured in the field, known minimum and maximum values can be set prior to LUT generation. (2) The selection of a cost/loss function can play a role in the inversion process. Many (i.e. >60) cost functions have been proposed to deal with error distributions (Leonenko et al., 2013a,b). However, Rivera et al. (2013) and Verrelst et al. (2014) showed that the use of different cost functions alone did not lead to optimized performance of LUT based inversion. (3) Instead of using the single best solution to the inversion problem, it is possible to use the mean or median of the n - best solutions (Darvishzadeh et al., 2011; Darvishzadeh et al., 2012; Verrelst et al., 2015b). (4) It has been shown that the addition of Gaussian noise can enhance the LUT inversion process (Richter et al., 2009; Richter et al., 2011; Verrelst et al., 2015b). Noise is inserted to account for uncertainties linked to the spectral measurements (i.e. instrument noise) and models (i.e. inability of the model to simulate reflectance) (Verrelst et al., 2015b). (5) The choice of specifically targeted wavelengths has been

shown to increase the accuracy of inversions (e.g. those wavelengths that have direct relationship to the variables under investigation) (Darvishzadeh et al., 2011).

Iterative numerical optimization, or curve fitting, is a conventional technique used to invert leaf and canopy RTMs (Jacquemoud et al., 1995; Jacquemoud et al., 2009; Kuusk, 1998; Zarco-Tejada et al., 2001; Liang et al., 2015; Verrelst et al., 2015b). The optimization consists of minimizing a cost function which quantifies/estimates the difference between the measured and estimated variables (i.e. the measured and modelled spectra) by sequentially iterating the variables of the RTM until the curves match as closely as possible (i.e. until the value of the cost function is minimized) (Verrelst et al., 2015b). The model parameter combination that makes up the solution to the matched spectra is considered the starting point/solution, and is thus considered to be the inverted parameters. Iterative numerical optimization algorithms are impractical for inverting large remote sensing datasets since they are computationally demanding (Verrelst et al., 2015b). Additional drawbacks of using iterative numerical optimization techniques in an operational setting are: (1) regularization techniques are required to achieve accurate results (Zarco-Tejada et al., 2001); however, this can be expected when using any inversion technique (as described above for LUT inversion by constraining the variables); and (2) numerical inversion using this approach can result in a local minima solution different from the global minimum (Liang, 2005; Verger et al., 2011). Common optimization algorithms used in remote sensing include the Nelder-Mead downhill simplex method (Nelder & Mead, 1965), which uses a gradient descent method, and the Levenberg-Marquardt algorithm (LMA), which uses a damped least squares curve fitting procedure (Levenberg, 1944; Marquardt, 1963; Morrison, 1960). Both have been used in various studies (e.g. Vohland et al., 2010; Hilker et al., 2017). Like LUT-based inversion, it is possible to

implement the previously mentioned regularization strategies when implementing iterative numerical optimization.

Overall strengths of physically-based RTMs and their inversion include: (1) they are full spectrum, (2) they can be generalized when correctly parameterized (e.g. Myneni et al., 2002), (3) they have the capability to produce multiple outputs (i.e. estimates of biochemical and biophysical variables that are not known), and (4) they can provide additional information about the uncertainty of the retrievals (through spectral residuals) (Verrelst et al., 2015b). Overall weaknesses include: (1) retrieval quality depends upon the formulation and parameterization of the RTM model, (2) RTM methods are complex and their inversion requires optimization, (3) the upper and lower limits of the variables constrict the model output, an approach that contradicts the physical approach (i.e., the prior or input data have influence the outcome of the model) (Baret & Buis, 2008), (4) like any modelling procedure, the inversion can be strongly affected by noise and measurement uncertainty (Verrelst et al., 2015b), and (5) processing power requirements are generally far greater than that of empirical modelling techniques, often rendering such models unrealistic for operational implementation (Verrelst et al., 2015b).

2.2.3.1.1. LMA numerical inversion and implementation

The iterative numerical optimization algorithm tested in this research was the Levenberg-Marquardt algorithm (LMA). LMA is known as a damped least squares method and is used to solve non-linear least squares curve-fitting problems. The LMA inversion method was chosen for three reasons: (1) at the time of commencing this research, it had not been used to invert the PROSAIL model, (2) a recent study showed that it can produce excellent results when inverting multi-angle reflectance data for biochemical variable estimation (Hilker et al., 2017), and (3) comparative studies have shown no real advantage to using a LUT over iterative optimization

methods, other than mapping speed and computation time (Vohland et al., 2010; Preidl & Doktor, 2011).

The Levenberg-Marquardt curve fitting algorithm functions through the combination of two minimization methods: (1) the gradient descent method, and (2) the Gauss-Newton method (Gavin, 2017). The gradient descent method, also known as the steepest descent method, is a general minimization method that iteratively updates the function's parameter values in a downhill direction, which is in a direction opposite to the gradient of the object function (Gavin, 2017). The gradient descent method tends to work well with problems with thousands of parameters and with problems with noncomplex objective functions (Lourakis, 2005; Madsen et al., 2004; Gavin, 2017). The Gauss-Newton method, on the other hand, minimizes the sum-of squares of the objective function. It assumes that the parameter space of the objective function is effectively quadratic when closest to the optimal solution (Bjorck, 1996; Gavin 2017). Finally, it typically converges much faster than the gradient descent method when the problem is moderate in size, by comparison (Marquardt, 1963; Gavin 2017).

The LMA incorporates both above methods into its functioning by switching adaptively (interpolating) between the two. For example, the gradient descent method is used when the function's parameter values are far from optimal, and the Newton-Gauss method is used when values are closer to optimal (Gavin, 2017). Like most fitting algorithms, LMA finds only the local minimum, which is not necessarily the global minimum, and so is susceptible to error if the initial parameter guesses are far from optimal. In this research, the LMA iterative numerical optimization approach was implemented as the method to invert the PROSAIL RTM. The LMA modelling approach can be seen below in Figure 14.

Figure 14 Iterative numerical optimization inversion approach using LMA and PROSAIL leaf-canopy RTM. The inversion was completed for each multi-angle spectral measurement. Parameters of the PROSAIL model were iteratively evaluated until the modelled and measured spectra matched as closely as possible (i.e. using a minimization function). The PROSAIL model parameters were then compared to the measured biochemical and biophysical variables using linear regression. Models were evaluated using r^2 and error metrics, such as RMSE

Part II: Field and Remote Sensing Studies

Chapter 3. Destructive and Non-destructive Field and Lab Measurement of Leaf and Canopy Chlorophyll Content Across an Arctic Bioclimatic Gradient

Abstract

The biochemical composition of canopy-dominant Western Arctic vegetation species was measured using destructive lab-based spectrophotometry. The measurement and characterization of dominant canopy Arctic species' pigment and non-pigment biochemicals were completed for calibration, parameterization, and validation of the empirical and physical modelling efforts presented later in this thesis. Mean field-based leaf chlorophyll content (LCC) was estimated based on the mass-weighted average of harvested and sorted canopy vegetation types taken at one of the field sites. This was statistically compared to non-destructive field-based handheld chlorophyll measurements taken across five field locations representing a latitudinal gradient between the years 2011 to 2013. A Genesis 10 UV-Vis spectrophotometer was used in a laboratory setting to measure total chlorophylls ($a+b$) and carotenoids for samples taken destructively of all dominant species to determine the typical per-species pigment values in $\mu\text{g}/\text{cm}^2$. Species wet leaf weights (mg/cm^2) were measured and compared to oven dried leaf weight (mg/cm^2) to determine the per-species equivalent water thickness (EWT). In addition, oven dried weights were used to determine the per-species dry matter content (mg/cm^2). Once representative biochemical values were obtained for each species, the total above ground phytomass was harvested in 99 random plots measuring 1 m^2 . All species' leaves were sorted and weighed. A weighted average using the per-species pigment values was used to find the average field-based leaf chlorophyll and carotenoid content in the 1 m^2 subplots. Non-destructive assessment of leaf chlorophyll content was measured

at the field sites using a Minolta SPAD-502 chlorophyll meter (SPAD). Relative SPAD measurements were converted into surface-based specific units of chlorophyll in $\mu\text{g}/\text{cm}^2$ using a linear consensus equation ($\text{Chlorophyll } (\mu\text{g}/\text{cm}^2) = (99 \cdot \text{SPAD}) / (144 - \text{SPAD})$). SPAD measurements were statistically compared to lab-based biochemical measurements using a standard one-tailed analysis of variance (ANOVA). Comparisons of means between sites were made with the Tukey post-hoc test. Results showed that there were no significant differences between the lab-based weighted leaf chlorophyll content values and the handheld non-destructive measurements taken in the Richardson Mountains (2014) when compared at the plot level ($p > 0.05$), thereby justifying the use of the SPAD data to represent all sites. The field-based chlorophyll measurements demonstrated a latitudinal gradient, from $\sim 40.7 \mu\text{g}/\text{cm}^2$ at the lowest latitude to $\sim 32.0 \mu\text{g}/\text{cm}^2$ at the highest latitude. Results also showed that statistically significant differences existed between the low and high latitude sites ($p \leq 0.05$) when compared at both the subplot and plot spatial scales.

3.1. Introduction

Quantification and assessment of vegetation biochemistry in remote sensing can typically be separated into two chemical groupings: pigment based constituents and non-pigment based constituents (Ustin et al., 2004; Kokaly et al., 2009; Ustin et al., 2009). The pigment biochemical constituents of plants include chlorophyll *a*, chlorophyll *b*, carotenoids, and anthocyanins (Balckburn, 2007; Ustin et al., 2009); non-pigment biochemicals include water, nitrogen, cellulose, and lignin (Kokaly et al., 2009). While leaf non-pigment biochemicals, such as nitrogen, lignin, and cellulose, have been recognized as being extremely important for ecosystem studies and monitoring (e.g. Kokaly et al., 2009), the following investigation focuses on the estimation of total leaf chlorophyll (*a+b*) content, carotenoid content, water content, and dry leaf matter weight of

various Arctic species using lab-based destructive and field-based non-destructive methods. The measurement and characterization of dominant Arctic species' pigment and non-pigment biochemicals were completed for calibration, parameterization, and validation of the empirical and physical modelling efforts (Chapters 5-7).

Total chlorophylls ($a+b$) play an important role in the conversion of solar radiation into stored biochemical energy through photosynthesis, a natural process that produces both oxygen and organic matter (Nelson & Yocum, 2006; Serrano et al., 2008; Croft et al., 2014). Chlorophyll concentrations limit the photosynthetic capacity of leaves and canopies and therefore the total chlorophyll content present within an ecosystem limits net primary production (NPP) (Richardson et al., 2002). Detection and measurement of total chlorophyll can further provide insight into plant disturbance and stress caused by changing environmental conditions (Gitelson et al., 2003; Sampson et al., 2003; Ustin et al., 2009; Richardson et al., 2002; Walker et al., 2016). Therefore, the retrieval of quantitative estimates of leaf and canopy chlorophyll content from remote sensing data can be considered important for understanding and monitoring ecosystems (Croft et al., 2014).

Carotenoid pigments are associated with photosynthesis, and are responsible for such processes as light harvesting, energy transfer, and photoprotection of chlorophyll pigments (Siefermann-Harms, 1987; Frank & Cogdell, 1996; Demmig-Adams, 1998; Ritz et al., 2000; Gitelson et al., 2002b; Young, 1991; Garrity et al., 2011). The total quantity of carotenoids within intact leaves is known to be associated with plant stress and photosynthetic capacity (Adams et al., 2002; Kirchgebnner et al., 2003; Munné-Bosch & Penuelas, 2003; Demmig-Adams & Adams, 1996; Munné-Bosch & Penuelas, 2003; Garrity et al., 2011). Since carotenoids are related to and respond to their environment, the ability to quantify their spatial distribution has the potential to enhance our understanding leaf and ecosystem processes such as photoprotection, photosynthetic

acclimation, and photosynthetic efficiency (Kokaly et al., 2009; Garrity et al., 2011). Pigment biochemicals, such as chlorophyll and carotenoids are increasingly being incorporated into leaf and canopy physical modelling approaches (e.g. PROSAIL, Jacquemoud et al., 2009 used in this research), and as such their measurement and retrieval represent crucial components to those efforts.

Water, a non-pigment biochemical, is typically the most abundant chemical found within vegetation in any environment as it constitutes nearly 40-80% of the volume of plant leaves (Shen et al., 2005; Kokaly et al., 2009; Mobasheri & Fatema, 2013). It is also one of the most important chemicals that control vegetation growth and the development of ecosystems (e.g. water is a limiting factor in ecosystem development, including the Arctic) (Kramer & Boyer, 1995). At the leaf level, water is essential for the preservation of leaf structure and shape, the regulation of temperature, and photosynthetic processes (Kokaly et al., 2009). Like both chlorophyll and carotenoids, spatiotemporal estimates of foliar and canopy water content can be used for ecosystem assessment and monitoring since plant stress can often be linked to water availability (Ustin et al., 1998; Kokaly et al., 2009). Foliar water content can be assessed using non-destructive methods, but first needs to be related to a measured quantity. For example, the equivalent water thickness (EWT) index can be implemented only through destructive sampling approaches (Bowyer & Danson, 2004). EWT also plays an important role in physical modelling since the reflectance of leaves and canopies is significantly impacted by the quantity of water contained within them (Kokaly et al., 2009; Olliger, 2011). Water is a major absorber of most wavelengths in the visible and especially in the near-infrared (NIR), resulting in reflectance attenuation in leaves and canopies (Olliger et al., 2011). Because of the large influence that water plays in leaf and canopy

reflectance, it is considered an important component of leaf and canopy RTMs (Jacquemoud et al., 2009).

The traditional destructive approach for estimating chlorophyll and carotenoids from leaves is through wet chemical methods that involve pigment extraction in organic solvents followed by spectrophotometric measurement (Gitelson et al., 2009). Laboratory based procedures can be difficult, time consuming, and not always practical to implement, especially when working in remote locations. Wet methods further entail the storage and transportation of time sensitive samples; chlorophyll degradation (along with other pigment biochemicals) typically begins once healthy leaves are removed from the plant (Ustin et al., 2009; Croft et al., 2014). Additional constraints are imposed by means of extraction/analysis of a given chemical; the estimation of foliar water and dry matter content requires the use of drying equipment and an accurate laboratory-grade balance. An alternative approach is field spectroscopy which has the potential to be efficient and non-destructive (Gitelson et al., 2009). *In situ*, field-based estimation of pigments is typically completed using measurements of reflectance or absorption values or vegetation indices (VIs). Reflectance is measured with a spectroradiometer, while sensors such as chlorophyll meters use a light source to measure leaf absorption. Non-destructive optical methods have been widely used for chlorophylls (Aoki et al., 1986; Buschmann & Nagel, 1993; Gitelson and Merzlyak, 1994a,b; 1996; Gitelson et al., 1996; Lichtenthaler et al., 1996; Blackburn, 1998a,b; Datt, 1998; Gamon & Surfus, 1999; Curren et al., 2001; Sims & Gamon, 2002; Richardson et al., 2002; Gitelson & Merzlyak, 2004; Gitelson et al., 2009), carotenoids (Gamon et al., 1990; Blackburn 1998a,b; Datt 1998; Gamon & Surfus 1999; Zur et al., 2000; Sims & Gamon, 2002; Gitelson et al., 2002b; Gitelson & Merzlyak, 2004; Gitelson et al., 2006; Gitelson et al., 2009),

and water content (Riano et al., 2005a,b; Danson & Bowyer, 2004; Wang & Yang 2009; Zhang et al., 2010; Zhang et al., 2012).

The reflectance characteristics of vegetation, and those of leaves, are related to the absorption features of the chemical compounds present within them (Blackburn, 2007; Ustin et al., 2008; Kokaly et al., 2009; Gitelson et al., 2009). Optical estimation of the biochemical constituents within vegetation is a complex task because leaf reflectance is strongly influenced by the numerous overlapping absorption features of these chemical bonds (e.g. C-O, O-H, C-H, and N-H bonds) (Curan, 1989; Siciliano et al., 2008). For instance, the absorption maxima of chlorophyll *a* when extracted in diethyl ether are centered at 430 nm and 662 nm, and chlorophyll *b* has absorption maxima located at 453 nm and 642 nm (Ustin et al., 2009). Carotenoids, on the other hand, absorb maximally at 451 nm and 470 nm (Du et al., 1998). When multiple pigments are present, identification and quantification of the individual biochemicals within leaves and canopies becomes more difficult to obtain from optical approaches alone (Buschmann et al., 1994; Siciliano et al., 2008; Ustin et al., 2009; Kokaly et al., 2009). Multiple scattering within the leaf structural components further complicates pigment retrievals (Ollinger, 2011). Empirically based optical methods can show a high degree of reliability when used in controlled laboratory settings (Gitelson et al., 2009) but can prove to be unreliable when used in naturally occurring environments, as optical methods are further complicated at the canopy scale where reflectance is confounded by variations in canopy configuration and background reflectance/absorption features (Ustin et al., 2009; Ollinger, 2011).

Some studies have quantified pigments in Arctic species at the field scale but studies along latitudinal gradients, such as in this research, are rare to nonexistent. Tieszen and Johnson (1968) reported pigment structures for four different species in northern Alaska. Chlorophyll values of 32

to 77 $\mu\text{g}/\text{cm}^2$ were reported, values that were said to be like alpine tundra and temperate grasslands. Tieszen (1970) compared chlorophyll content and leaf structure (i.e. leaf thickness) in Arctic and alpine grasses, demonstrating similar chlorophyll quantities and that Arctic plants exhibited low chlorophyll *a/b* ratios but on average thicker leaves than alpine sites. Tieszen (1972) investigated the seasonal production of chlorophyll at Barrow, Alaska finding that peak chlorophyll production typically occurred at about July 25th. Early spectrophotometry studies such as the three above that used extinction coefficients from Arnon (1949) were not correct; Lichtenthaler (1987) determined new extinction coefficients and these widely accepted values were used in this research.

There exists a gap in the literature in reporting of regional values of plant biochemical quantities, at the ecosystem scale and across species. Ground-based measurements of biophysical and biochemical vegetation variables can be considered important for calibration and validation of empirical reflectance-based modelling efforts and for parametrization and validation of physically-based radiative transfer models. Furthermore, species-based and ground/canopy-based biochemical measurements provide a baseline from which future assessments can be compared.

The objectives of this study were fourfold: (1) to destructively (i.e. through lab-based spectrophotometry and oven drying) characterize the average pigment biochemical (chlorophylls and carotenoids) and non-pigment biochemical (water and leaf dry matter) content of the dominant Arctic tundra vegetation species found within a representative field site for the purpose of providing quantitative ecophysiological data for empirical and physical model parametrization, calibration, and validation; (2) to determine subplot-scale (1 m^2) mean leaf chlorophyll content using a destructive weighting procedure coupled with the spectrophotometrically derived species values; (3) to statistically compare the destructive mean weighted leaf chlorophyll content measurements to non-destructive hand-held instrument-based leaf chlorophyll measurements

taken across five field locations at the subplot-scale; and (4) compare the mean plot-based ($>1 \text{ m}^2$) leaf chlorophyll content measurements across a latitudinal gradient.

3.2. Materials and Methods

3.2.1. Study sites and sampling dates

Non-destructive field measurement of chlorophyll was conducted at all study sites described in Chapter 2. Destructive vegetation sampling for lab-based chlorophyll measurement was conducted at the Richardson Mountains site along the Dempster Highway. Figure 15 shows some example field photos for this site. The Richardson Mountains site is situated in alpine terrain and is thus often cloudy. Photos below demonstrate typical ground terrain (i.e. patterned ground) and vegetation canopies (i.e. shrubs and tussocks). It should be noted that all photos depicting vegetation show the beginning of autumn senesce (approximately August 18th); sampling of vegetation biochemistry occurred before the onset of autumn senesce (discussed below).

The Richardson Mountains field site was selected as a representative example of low-latitude heterogeneous (i.e. multi-species) tundra vegetation and because it was accessible by road and relatively close to the Aurora Research Institute (ARI) laboratory facilities in Inuvik, NT. Proximity to a lab is considered necessary for sampling of plant pigments since chlorophylls degrade when foliage is removed from the plant (Gitelson et al., 2009; Croft et al., 2014). All other field sites were in remote areas where destructive chemical sampling was not practical (e.g. Banks Island), and as such, *in situ* measurement of chlorophyll using handheld instrumentation was considered the best option in these locations.

Figure 15 Richardson Mountains (2014) field site. Clockwise from top: (1) typical cloudy conditions and terrain, (2) Dempster Highway and view of a typical sample site, (3) patterned ground areas were included in sample sites, (4) typical shrub (e.g. tealeaf willow and dwarf birch) and tussock canopy (e.g. cotton grass).

3.2.2. Destructive sampling: Spectrophotometry and weighted averaging

Destructive field sampling was conducted between July 20th and August 5th, 2014 using the dominant (most common) species found within the study area that were deemed to make up the largest portion of the vegetation canopy. Species included: *Vaccinium vitis-idaea* var. *minus*

(lingonberry), *Arctostaphylos uva-ursi* (bearberry), *Vaccinium uliginosum* (blueberry), *Rubus chamaemorus* (cloudberry), *Petasites frigidus* var. *frigidus* (Arctic sweet coltsfoot), *Carex aquatilis* (water sedge), *Eriophorum vaginatum* (cotton grass), *Betula nana* (dwarf birch), *Salix pulchra* (tealeaf willow), *Rhododendron tomentosum* (northern Labrador tea), *Sphagnum* (peat moss), and *Empetrum nigrum* (crowberry). Random samples were harvested for each species across all field plots at 50 m intervals along 250 m transects. Plot location was recorded with a handheld Trimble Juno GPS unit (accurate to ~3 m). In total 30 samples were collected and processed for each species across all subplots, amounting to 360 samples in total. When possible, the entire plant was removed from the ground to preserve the leaf structure. A wide variety of leaf/plant conditions (different stages of development) were sampled to account for leaf chlorophyll content variability. Samples were immediately wrapped in tinfoil, placed in a cooler with ice, and within 3 hours transported to the freezer at ARI in Inuvik. Samples were processed as quickly as possible over the next few days mindful of pigment/chlorophyll degradation.

Leaf pigment extraction with organic solvents and spectrophotometric determination in solution is required for pigment analysis with wet chemical methods (e.g. Lichtenthaler & Wellburn, 1983; Lichtenthaler, 1987; Lichtenthaler & Buschmann, 2005; Gitelson et al., 2009). Leaf pigments were analyzed as described by Gitelson et al. (2009) (Gitelson & Merzlyak 1994a,b; Gitelson et al., 2001; Gitelson et al., 2002b; Merzlyak et al., 2008; Steele et al., 2009). A surface area of 2 cm² was cut from the leaves and ground with a mortar and pestle in 80% acetone. Small leaves/needles were placed in a small template with a 2 cm² cut-out to find a known surface area. The species homogenates were centrifuged for 20 minutes at 5000 x gravity. The resulting extracts were immediately assayed spectrophotometrically with a Genesis 10 UV-Vis Spectrophotometer with a spectral range of 190 to 1100 nm (Thermo Fisher Scientific Inc. Waltham, MA, USA). Specific

absorption coefficients for chlorophyll *a*, chlorophyll *b*, and total carotenoids reported by Lichtenthaler (1987) were used.

The Beer-Lambert law is the foundation for the spectroscopic quantification of pigments in solvents. It defines the absorbance of a solution with respect to the specific light absorption characteristics (i.e. specific wavelengths) of the dissolved compound present (Lichtenthaler & Buschmann, 2005). When multiple pigments/compounds exist within homogenate, the standard Beer-Lambert law equations used to quantify individual compounds must be altered to account for the absorption complexities caused by the various compounds present (Lichtenthaler & Buschmann, 2005). Because the homogenate is always the sum of the multiple pigments found within the leaf sample, the absorbance of the homogenate is expressed as the sum of the multiple absorbances for the various pigment biochemicals present (Lichtenthaler & Buschmann, 2005). The determination of chlorophyll *a*, chlorophyll *b*, and total carotenoids ($x+c$ = xanthophylls and carotenes) concentration in acetone with 20% water has been given by Lichtenthaler (1987) and Lichtenthaler and Buschmann (2005), where pigment concentrations are given in $\mu\text{g/ml}$:

$$\text{Chlorophyll}_a (\mu\text{g/ml}) = 12.25 A_{663.2} - 2.79 A_{646.8} \quad (5)$$

$$\text{Chlorophyll}_b (\mu\text{g/ml}) = 21.50 A_{646.8} - 5.10 A_{663.2} \quad (6)$$

$$\text{Carotenoids}_{(x+c)} (\mu\text{g/ml}) = (1000 A_{470} - 1.82 C_b - 85.02 C_b)/198 \quad (7)$$

Measurements of $\mu\text{g/ml}$ were later converted to $\mu\text{g/cm}^2$ using the known leaf surface areas. It should be noted that the concentration of chlorophyll *a*, chlorophyll *b*, and total carotenoids ($x+c$) can be quantified using different reference systems. Common reference systems used for leaf pigments include $\text{mg chlorophyll } a+b/\text{m}^2 \text{ leaf area}$ (or $\mu\text{g/cm}^2 \text{ leaf area}$), $\mu\text{g chlorophyll } a+b/\text{mg dry leaf weight}$, and $\text{mg chlorophyll } a+b/\text{g fresh leaf weight}$ (which is less suitable than dry weight)

(Lichtenthaler & Buschmann, 2005). A reference system of $\mu\text{g}/\text{cm}^2$ was used because of its prevalence within the remote sensing literature (e.g. Darvishzadeh et al., 2008a; Croft et al., 2014; Jay et al., 2016) and because of its use within the PROSPECT and PROSAIL RTMs (Jacquemoud et al., 2009).

Leaf water content analysis was completed by clipping a known area of each species' leaves (e.g. 1 cm^2 using a template), weighing them (fresh), oven drying the samples for ~ 24 hours at $\sim 75^\circ$, and weighing them on an Ohaus Adventurer Pro Analytical Balance ($\pm 0.0002 \text{ g}$). Each of the species were sampled 30 times using samples that were considered matched pairs with the samples used for the pigment analysis (i.e. samples were selected based on similar condition). From the various leaf water indices in the literature (Wang et al., 2009; Mobasheri & Fatemi, 2013), Full Moisture Content (FMC) and Equivalent Water Thickness (EWT) are perhaps the most widely used (Mobasheri & Fatemi, 2013). Since EWT is used in the PROSAIL model, and it has been shown to have higher correlation with leaf spectral parameters than FMC (Bowyer & Danson, 2004; Shen et al., 2005), it was selected for this study. EWT is the weight of water per unit area of leaf and is calculated using Equation 8:

$$EWT = (FW - DW / A) (g \cdot \text{cm}^2) \quad (8)$$

where FW is the leaf fresh weight, DW is the leaf dry weight, and A is the leaf surface area (Bowyer & Danson, 2004).

The averaged chlorophyll, carotenoid, and EWT measurements per species were extrapolated to the average expected field conditions using a destructive weighting procedure. At each of the Richardson Mountains (2014) transects, 99 subplots measuring 1 m^2 were harvested. At each transect (Figure 10, Chapter 2), 5 subplots were used as representative examples of the expected leaf-canopy conditions. All aboveground phytomass (leaves and stems), including the very top

layer of green sphagnum was clipped and removed. Each plot's vegetation was then sorted by species; all woody materials were removed in the process. Total wet canopy leaf weight was measured and samples were subsequently oven dried (~48 hours at ~75°) to determine the total dry canopy leaf weight. The averaged lab measured pigment and non-pigment values were then applied to the harvested plots using a weighting based on the percentage of the plant species' weights that occupied the subplot/canopy, thus providing an averaged measure of pigment and non-pigment biochemical values across the canopy based on actual occurrence/abundance.

3.2.3. Non-destructive leaf chlorophyll measurement using the SPAD optical instrument

Non-destructive instrument-based chlorophyll measurements were taken between 2011 to 2013 as follows: (1) July 18th to July 29th, 2011, Herschel Island, YT; (2) July 10th to July 20th, 2012, Banks Island, NT; (3) July 25-26th, 2012, Richards Island, NT, (4) July 24th, 2012 Tuktoyaktuk, NT, (5) July 25th to August 4th, 2013, Richards Island, NT, and (6) July 18th to July 22nd, 2013 Richardson Mountains, YT/NT. The locations of the sampled field plots and ecophysiological description of each field site can be found in Chapter 2. They were completed before the destructive measurements described above because it was not possible to conduct both in the same season (i.e. instrument availability).

Measurements were taken with a Minolta SPAD-502 chlorophyll meter (Minolta Camera Co. Osaka, Japan). It performs quick measurements of leaf chlorophyll content *in situ* without damaging the leaf, thus making it ideal for non-destructive measurement in remote locations. SPAD values are a unit-less measure expressing the relative amounts of chlorophyll in leaves by measuring transmittance in the red (650 nm) and NIR (940 nm) wavelength regions using a calibrated light source that radiates through the leaf sample (Konica-Minolta, 2009). This instrument is commonly used to characterize chlorophyll concentration in plant species (e.g.

Dwyer et al., 1991; Markwell et al., 1995; Campbell et al., 1990; Haboudane et al., 2002; Darvishzadeh et al, 2012; Cerovic et al., 2012). The SPAD signal is transformed into proprietary index units called SPAD units using the equation (9):

$$f(l_o, l) = \log[l_{(940)}/l_{o(940)}] - \log[l_{(650)}/l_{o(650)}] \quad (9)$$

Where l_o are signals without the leaf sample, and l is the signal with the leaf sample present in the leaf clip at the given wavelengths (nm). The SPAD measures an area of 2 mm by 3mm and is capable of measuring leaves with a maximum thickness of 1.2 mm ((Konica-Minolta, 2009).

At each of the 2011 to 2013 field sites, plots measuring 90 m by 90 m were established within various vegetation assemblages that were distinct enough to be distinguished from medium resolution optical imagery (e.g. CHRIS/PROBA). It should be noted that the Richardson Mountains plots sampled in 2013 were not coincident to those plots sampled in 2014. Samples were taken in the centre of these distinct vegetation assemblages. Each of the field plots was divided into three equally spaced transects; seven equally spaced subplots measuring 1 m² were positioned along each transect. Within each of the subplots a total of 10 SPAD readings were taken and averaged to produce one measurement of average leaf chlorophyll content. Samples of the dominant species were randomly chosen, in-line with those destructively sampled as described above. A full range of leaf conditions was measured to produce an accurate account of leaf chlorophyll content variability; fully senescent vegetation was not measured. Species with difficult to measure leaf morphologies (e.g. crowberry and peat moss) were sampled by either placing several needles on the sensor or by clipping a small flat measurable surface. Figure 23 (Chapter 4) shows a diagram of the plot-based sampling technique used at all the field sites.

There exists substantial literature on the characteristics of various chlorophyll meters, with repeated attempts to produce a reliable calibration curve for accurate quantitative estimates of leaf

chlorophyll (Cerovic et al., 2012). Measurements are typically affected by leaf anatomical characteristics, such as thickness, fresh mass per unit area (succulence), dry mass per unit area, water content, an excess of a specific biochemical (e.g. chlorophyll), cuticle reflectance, the presence of palisade and spongy tissue, and proportions of veins in the leaf (Marenco et al., 2009; Yamada & Fujimura, 1991; Uddling et al., 2007; Imanishi et al., 2010). Essentially, all anatomical/morphological differences between specimens can confound readings, or rather, conversion of the proprietary values into actual biochemical values (e.g. $\mu\text{g}/\text{cm}^2$). Most of these anatomical/morphological effects can be grouped under the concept of sieve effects (i.e. transmittance larger than in a homogenous sample) and detour effects (i.e. absorption larger than in a homogenous sample) (Vogelmann, 1993; Uddling et al., 2007; Cerovic et al., 2012).

It is therefore recommended that the sensor be calibrated for the plant species of interest within the environment of interest by extractive wet chemistry methods (Cerovic et al., 2012). Unfortunately, the SPAD measurements taken in the 2011-2013 field seasons were not calibrated with the destructive measurements due to the remoteness of the field sites. Nor were the destructive measurements taken in the 2014 field season calibrated to the instrument due to lack of simultaneous equipment availability. This may result in increased uncertainty/error as discussed in Chapter 8. Instead, a linear calibration function, or consensus equation (Cerovic et al., 2012), was used to convert the SPAD values to actual measurements of chlorophyll in $\mu\text{g}/\text{cm}^2$. The consensus equation (10) is:

$$\text{chlorophyll } (\mu\text{g}/\text{cm}^2) = (99 \times \text{SPAD}) / (144 - \text{SPAD}) \quad (10)$$

It was developed by Cerovic et al. (2012) by taking published calibration curves from seven studies (although none were for Arctic vegetation) and determining the best linear fit (Markwell et al.,

1995; Richardson et al., 2002; Cartelat et al., 2005; Uddling et al., 2007; Marengo et al., 2009; Coste et al., 2010; Ling et al., 2011a,b).

The converted SPAD values ($\mu\text{g}/\text{cm}^2$) for all sites were statistically compared to the destructive lab-based measurements from the Richardson Mountains site using a one-way analysis of variance (ANOVA) to determine if the sampled means were significantly different. A finding of no significant difference would provide some confidence that measured SPAD values of the 2011-2013 field seasons reflected the 2014 quantities measured in the lab. Lastly, PAI was destructively measured at each of the plots (Chapter 4 provides details about where these data come from, as they were part of a broader set of measurements) and compared to harvested leaf-canopy biochemical values.

3.3. Results

3.3.1. Destructive vegetation sampling: Spectrophotometric pigment measurement

The lab-based spectrophotometric results for the twelve Arctic species are shown in Table 1. Values of total chlorophylls ($a+b$) ranged from $10.5 \mu\text{g}/\text{cm}^2$ for peat moss up to $57.2 \mu\text{g}/\text{cm}^2$ for Labrador tea. Average total chlorophyll content over all species was $37.5 \mu\text{g}/\text{cm}^2$. These values do not differ substantially from the average value of $38 \mu\text{g}/\text{cm}^2$ reported by Tiezen and Johnson (1968). This low level of chlorophyll is likely related to the low light intensity of the region. Figure 16 shows the pigment value ranges for the various sampled species. A high degree of pigment variability can be seen amongst and between the plant species and is likely attributable to the sampling of a wide variety of vegetation conditions (intra-species) and the various leaf-structures and pigment adaptations (inter-species).

Figure 16 Lab-based measurements of chlorophyll and carotenoid quantities for all species (common names shown). Boxplots show the interquartile range with factor of 1.5; outliers are displayed with a +.

The ratio of chlorophyll *a* to chlorophyll *b* (*a/b*) has been shown to be an indicator of the pigment structures and light adaption of the photosynthetic apparatus with leaves (i.e. light adaptation) (Lichtenthaler et al., 1981; Lichtenthaler & Buschmann, 2005; Yamori et al., 2016). Shade(d) plants/leaves possess chlorophyll *a/b* ratios that are lower than those of sun-exposed

plants/leaves (Licthenthaler et al., 1982, 1984; Lichtenthaler & Buschmann, 2005). The overall chlorophyll *a/b* ratios for all species can be seen in Table 1. The typical values found across the species measured ranged from 2.1 for sphagnum to 5.1 for Arctic sweet coltsfoot. Although these are Arctic species, the average value of ~3.5 reported here is comparable to those reported by Lichtenthaler and Buschmann (2005) for fully developed sunlit leaves in broad-leaved deciduous trees (e.g. beech and poplar). Average values reported by Tiezsen and Johnson (1968) differ from those reported here, where their highest ratio values were ~2.5 for *Salix pulchra*. The plotted relationship between chlorophyll *a* and chlorophyll *b* for all species is given in Figure 17. The relationship of 3/1 is observable, indicating that most species sampled were predominantly sunlit leaves (i.e. low and open canopies). These values are not surprising considering the configuration of tundra canopy.

Table 1 Averaged chlorophyll and carotenoid values for all destructively sampled species.

<i>Species</i>	<i>Chl a</i> ($\mu\text{g}/\text{cm}^2$)	<i>Chl b</i> ($\mu\text{g}/\text{cm}^2$)	<i>Chl a+b</i> ($\mu\text{g}/\text{cm}^2$)	<i>x+c</i> ($\mu\text{g}/\text{cm}^2$)	<i>Chl a/b</i> ($\mu\text{g}/\text{mg}$ <i>ww</i>)*	<i>x+c</i> ($\mu\text{g}/\text{mg}$ <i>ww</i>)	<i>Chl a/b</i> ($\mu\text{g}/\text{mg}$ <i>dw</i>)*	<i>x+c</i> ($\mu\text{g}/\text{mg}$ <i>dw</i>)	<i>a/b</i>	<i>(a +b)/</i> <i>(x+c)</i>
<i>Vaccinium vitis-idaea</i> var. <i>minus</i> (Lingonberry)	37.88	12.25	50.12	14.25	1.11 (45.10)	0.32 (45.10)	5.89 (8.5)	1.68 (8.5)	3.15	3.52
<i>Arctostaphylos uva-ursi</i> (Bearberry)	28.29	7.27	35.57	11.14	1.13 (31.67)	0.35 (31.67)	4.18 (8.5)	1.31 (8.5)	3.87	3.19
<i>Vaccinium uliginosum</i> (Blueberry)	31.46	8.77	38.89	11.73	1.96 (20.96)	0.56 (20.96)	6.27 (6.2)	1.89 (6.2)	3.61	3.32
<i>Rubus chamaemorus</i> (Cloudberry)	32.11	9.41	41.52	9.99	2.45 (17.16)	0.58 (17.16)	5.13 (8.1)	1.23 (8.1)	3.43	4.16
<i>Petasites frigidus</i> var. <i>frigidus</i> (Arctic sweet coltsfoot)	20.35	5.55	25.91	5.62	1.08 (24.39)	0.23 (24.39)	4.47 (5.8)	0.97 (5.8)	5.06	4.61
<i>Carex aquatilis</i> (Water sedge)	28.42	8.16	36.58	10.70	1.30 (27.57)	0.39 (27.57)	5.63 (6.5)	1.65 (6.5)	3.38	3.42

<i>Eriophorum vaginatum</i> (Cotton grass)	31.17	9.36	40.53	16.43	0.92 (44.69)	0.37 (44.69)	4.77 (8.5)	1.93 (8.5)	3.36	2.47
<i>Betula nana</i> (Dwarf birch)	24.22	6.60	30.82	9.43	1.47 (20.97)	0.45 (20.97)	3.63 (8.5)	1.11 (8.5)	3.72	3.23
<i>Salix pulchra</i> (Tealeaf willow)	37.35	8.46	45.81	13.79	1.64 (27.62)	0.50 (27.62)	4.16 (11.0)	1.25 (11.0)	4.46	3.32
<i>Rhododendron tomentosum</i> (Northern Labrador tea)	41.03	16.16	57.19	17.79	1.75 (34.06)	0.52 (34.06)	2.87 (19.9)	0.89 (19.9)	2.56	3.21
<i>Sphagnum</i> (Peat moss)	7.09	3.39	10.48	3.33	0.12 (90.37)	0.04 (90.37)	1.04 (10.1)	0.33 (10.1)	2.10	3.15
<i>Empetrum nigrum</i> (Crowberry)	27.46	9.29	36.75	23.03	0.92 (40.42)	0.57 (40.42)	2.08 (17.7)	1.30 (17.7)	2.93	1.60

*Average wet and dry weight per species listed below for reference (mg/cm²).

In addition to the interpretation of chlorophyll *a/b* weight ratio for light response, the weight ratio of total chlorophylls to total carotenoids $(a+b)/(x+c)$ can provide a means for assessing the greenness of leaves and canopies (Lichtenthaler & Buschmann, 2005). According to Lichtenthaler (2001), the ratio of total chlorophylls to total carotenoids of plants typically lies between 4.2 and 5.0 for sun leaves and between 5.5 and 7.0 for shade leaves. $(a+b)/(x+c)$ ratios that are lower are considered an indicator of senescence, plant stress, and damage to the photosynthetic apparatus (leaves); consequently, a lower $(a+b)/(x+c)$ ratio is due to the faster breakdown of chlorophylls than carotenoids (Lichtenthaler & Buschmann, 2005). Senescent vegetation will typically exhibit $(a+b)/(x+c)$ values of 3.5, but values may be as low as 2.5 as senescence advances (Lichtenthaler & Buschmann, 2005). The $(a+b)/(x+c)$ ratio values obtained in this study were between 1.6 for crowberry and as high as 4.6 for Arctic sweet coltsfoot. The lower values fall in the range reported by Tiezsen and Johnson (1968) of ~1.5 to 2.5. Figure 17 shows the relationship/ratio of total chlorophylls $(a+b)$ to carotenoids $(x+c)$ for all species. The heteroscedasticity evident in Figure

17 (bottom left and right) is due to the differing biochemical compositions/ratios of the species sampled (i.e. all species results were pooled).

Figure 17 Chlorophyll *a* vs chlorophyll *b* for all species sampled (top left) and for averaged species values (top right). Total chlorophyll vs. carotenoids for all species (bottom left) and total averaged chlorophyll vs. carotenoids values for all species (bottom right). The observed heteroscedasticity is due to the pooling of all species with varying degrees of chlorophyll/carotenoid ratios. In the bottom right, the outlier represents a species (crowberry) with high carotenoid content.

3.3.2. Equivalent water thickness (EWT)

The equivalent water thickness (EWT) values are shown in Table 2 below. EWT values were not matched to each of the chlorophyll/carotenoid samples due to the destructive nature of the spectrophotometry. The mean EWT for all species combined was approximately $\sim 0.03 \text{ g/cm}^2$.

Table 2 Averaged EWT (moisture) values for all vegetation types. Fresh leaf and dried leaf weights are shown.

<i>Species</i>	<i>WW</i> (g/cm ²)	<i>Min</i> (g/cm ²)	<i>Max</i> (g/cm ²)	<i>Std.</i> <i>Dev.</i> (g/cm ²)	<i>DW</i> (g/cm ²)	<i>Min</i> (g/cm ²)	<i>Max</i> (g/cm ²)	<i>Std.</i> <i>Dev.</i> (g/cm ²)	<i>EWT</i>
<i>Vaccinium vitis-idaea</i> var. <i>minus</i> (Lingonberry)	0.045	0.035	0.054	0.005	0.009	0.007	0.010	0.001	0.037
<i>Arctostaphylos uva-ursi</i> (Bearberry)	0.032	0.025	0.038	0.004	0.009	0.006	0.012	0.001	0.023
<i>Vaccinium uliginosum</i> (Blueberry)	0.021	0.016	0.024	0.002	0.006	0.005	0.010	0.001	0.015
<i>Rubus chamaemorus</i> (Cloudberry)	0.017	0.014	0.021	0.002	0.008	0.006	0.011	0.001	0.009
<i>Petasites frigidus</i> var. <i>frigidus</i> (Arctic sweet coltsfoot)	0.024	0.018	0.035	0.004	0.006	0.004	0.007	0.001	0.019
<i>Carex aquatilis</i> (Water sedge)	0.028	0.013	0.038	0.006	0.007	0.006	0.008	0.001	0.021
<i>Eriophorum vaginatum</i> (Cotton grass)	0.045	0.031	0.058	0.007	0.009	0.007	0.012	0.001	0.036
<i>Betula nana</i> (Dwarf birch)	0.021	0.018	0.023	0.001	0.009	0.006	0.012	0.001	0.013
<i>Salix arctica</i> (Arctic willow)	0.028	0.019	0.033	0.003	0.011	0.009	0.014	0.002	0.017
<i>Rhododendron</i> <i>tomentosum</i> (Northern Labrador tea)	0.034	0.023	0.045	0.007	0.020	0.015	0.023	0.002	0.014
<i>Sphagnum</i> (Peat moss)	0.090	0.052	0.107	0.012	0.010	0.008	0.013	0.002	0.080
<i>Empetrum nigrum</i> (Crowberry)	0.040	0.034	0.046	0.003	0.018	0.015	0.021	0.001	0.023
All Species Mean	0.035	0.013	0.107	0.020	0.010	0.004	0.023	0.004	0.026
EWT Min	-	-	-	-	-	-	-	-	0.009
EWT Max	-	-	-	-	-	-	-	-	0.080
EWT Std. Dev.	-	-	-	-	-	-	-	-	0.019

Minimum EWT values were approximately 0.01 g/cm^2 , whereas maximum values were in the 0.08 g/cm^2 range. EWT values for Arctic vegetation have not been reported in the literature; however, they have been reported for similar species. For example, Mobasheria and Fatemi (2013) reported willow values of 0.01 g/cm^2 compared to 0.02 g/cm^2 found here for Arctic willow. The highest values obtained in this research are for sphagnum (0.08 g/cm^2), due to its ability to hold moisture better than most other species. The values obtained for the 2014 Richardson Mountains field plots are in-line with values commonly used in the PROSPECT leaf model of 0.00 to 0.05 g/cm^2 (Darvishzadeh et al., 2008a).

3.3.3. Comparison of spectrophotometry to leaf/canopy weight and PAI

The destructive plant area index (PAI_d) values (m^2/m^2) were compared to the oven dried canopy weights (g/m^2) harvested at the subplot scale. In total, 99 plots were sampled. Overall, there was a somewhat weak relationship ($r^2=0.45$) between PAI_d and total dry vegetation weight (g/m^2). This was partially due to the presence of woody components and senescent vegetation. Indeed, when the vegetation was sorted, and the woody biomass and senescent vegetation were excluded, the relationship between PAI_d and total dry leaf weight (g/m^2) improved ($r^2=0.63$). Figure 18 shows the relationship between PAI_d and dried whole-canopy and canopy-leaf weights. These relationships show that PAI measurements could be used as an approximate measure for green phytomass in tundra ecosystems (i.e. the total mass of all green plant materials per unit area). Following this, all subsequent PAI measures were done using only the green portions of vegetation (see Chapter 4).

Figure 18 Measured PAI_d vs. total dried canopy weight and total dried leaf weight (woody materials removed).

Fresh leaf weights had poorer relationships with total measured chlorophyll and carotenoids ($r^2=0.14$ and $r^2=0.32$, respectively) than dried leaf weights ($r^2=0.48$ and $r^2=0.64$, respectively) (Figure 19). It should be noted that when sphagnum was removed, relationships improved – a result that is due to its overall low pigment values (see Chapter 8).

Figure 19 Leaf wet and dry weights (mg/cm²) vs. total chlorophyll content (µg/cm²) (left column) and leaf wet and dry weights (mg/cm²) vs. total carotenoid content (µg/cm²) (right column).

3.3.4. Field scale weighted chlorophyll and carotenoid values

For each of the plots in the Richardson Mountains (2014) study area the mean leaf chlorophyll, carotenoid, and EWT values were estimated using a weighted average based on the mass of each species in each plot to derive estimates at the field scale (Table 3).

Table 3 Weighted values of canopy chlorophyll and carotenoid content. EWT values included for reference.

<i>Weighted Canopy Content</i>	<i>n</i>	<i>Mean</i> (µg/cm ²)	<i>Min</i> (µg/cm ²)	<i>Max</i> (µg/cm ²)	<i>Std.</i> <i>Dev.</i>
Total Carotenoids (x+c)	99	14.6	9.1	19.4	2.1
Total Chlorophyll (a+b)	99	40.7	31.0	50.5	3.8
Equivalent Water Thickness	99	0.03	0.01	0.04	0.006

Canopy averaged leaf chlorophyll content (CCC) and canopy carotenoid content were estimated by multiplying the green PAI_d values by the weighted per-plot biochemical values (e.g. chlorophyll and carotenoids measured in µg/cm²) to obtain representation of plot-scale total chlorophyll and carotenoids value in g/m² (Darvishzadeh et al., 2008a). CCC values scale much higher than the leaf biochemical content values since they are representative of the canopy and not the leaf;

nevertheless, CCC may be considered a more accurate spatial representation of canopy level biochemistry since it takes the cover/leaf area into account (Darvishzadeh et al., 2008a). For example, a site with sparse vegetation but high readings of chlorophyll may be misrepresented by the high values measured within the leaf. When CCC is compared to dried canopy weight a relatively good relationship is observed ($r^2=0.47$); however, this relationship improves when compared to total dry leaf weight ($r^2=0.62$) (Figure 20). When carotenoid canopy content is compared to dried canopy weight and then dried leaf weight similar relationships are observed ($r^2=0.50$ and $r^2=0.60$, respectively) (Figure 20). Although the canopy values for carotenoids were calculated, only the leaf scale values were retained for use in parameterization of the leaf-based physical model (PROSPECT). Canopy chlorophyll content values ranged between 0.04 to 0.99 g/m^2 whereas canopy carotenoid values ranged from 0.02 to 0.37 g/m^2 .

Figure 20 Dried vegetation weights (leaf and canopy) vs. canopy chlorophyll content (CCC) (top) and canopy carotenoids content (bottom). The observed heteroscedasticity is due to the pooling of all species with varying degrees of chlorophyll and carotenoid content and differing leaf weights.

3.3.5. Comparison of chlorophyll values from lab spectrophotometry with field-based instrument measurements

A latitudinal comparison between the destructive chlorophyll sampling and the converted SPAD values can be seen in Figure 21. Across the field sites there exists a latitudinal gradient of average measured leaf chlorophyll values, progressing from the highest values encountered at lower latitudes, $40.7 \mu\text{g}/\text{cm}^2$ in the Richardson Mountains (2014), to the lowest average recorded value of $32.0 \mu\text{g}/\text{cm}^2$ found at the highest latitudes (Banks Island). However, it should be noted that the variance in leaf chlorophyll values at each site was large enough that some values were similar between higher and lower latitude sites. For example, the highest latitude site, Banks Island, had some leaf chlorophyll measurements that were in the same range as sites at lower latitudes such as Richards Island. The lower chlorophyll values recorded at Banks Island may be due to the onset of winter senescence and may not necessarily reflect peak chlorophyll levels.

Figure 21 Total leaf chlorophyll content (LCC) vs. latitude. Each of the study sites is shown in a latitudinal gradient beginning in the most southern sites and progressing to the most northerly sites. A trend, plotted using median values, is shown.

An ANOVA statistical comparison of leaf chlorophyll content measurements was completed to compare the 2014 destructive leaf chlorophyll content values from the Richardson Mountains site to the 2011-2013 non-destructive SPAD leaf chlorophyll content values measured at the remaining sites. The descriptive statistics for the subplot leaf chlorophyll content measurements are shown in Table 4. The results of subplot scale ANOVA are given in Table 5. They showed a statistically significant difference in average leaf chlorophyll between the field sites ($p > 0.05$, $F = 32.3$). Tukey's post-hoc test (Table 6) showed a statistically significant difference between the destructive and SPAD chlorophyll measurements for the Richardson Mountains site. This may be due to incorrect conversion of SPAD values or to the differences in date and year of the destructive vs. SPAD measurements. These differences may have also been due to the variability of the subplot measurements.

Table 4 Descriptive statistics for converted SPAD values ($\mu\text{g}/\text{cm}^2$) for all field sites for subplot data. Richardson Mountains (2014) destructive measurement values are also included. Plots with zero values excluded (no leaf measurements taken).

<i>Chlorophyll ($\mu\text{g}/\text{cm}^2$)</i>					<i>95% Confidence Interval</i>			
<i>Site/Location (#)</i>	<i>n</i>	<i>Mean</i>	<i>Std. Dev.</i>	<i>Std. Err.</i>	<i>Lower</i>	<i>Upper</i>	<i>Min</i>	<i>Max</i>
1. Herschel Island 2011	693	34.9	6.5	0.2	34.4	35.4	19.0	54.8
2. Banks Island 2012	520	32.0	7.1	0.3	31.4	32.6	12.6	49.5
3. Richards Island 2012	34	34.9	5.2	0.9	33.1	36.7	24.8	45.9
4. Richards Island 2013	162	33.5	6.1	0.5	32.6	34.4	19.0	53.1
5. Tuktoyaktuk 2012	52	34.1	4.2	0.6	32.9	35.2	25.8	44.0
6. Richardson Mountains 2013	225	36.1	6.1	0.4	35.3	36.9	22.2	55.3
7. Richardson Mountains 2014	99	40.7	3.8	0.4	39.9	41.5	31.0	50.4
Total	1785	34.4	6.7	0.2	34.1	34.7	12.6	55.3

Table 5 ANOVA results for leaf chlorophyll content comparisons by field site at the subplot scale. Results are significant at the 0.05 level.

<i>Chlorophyll</i>	<i>Sum of squares</i>	<i>Degrees of freedom</i>	<i>Mean square</i>	<i>F</i>	<i>Significance</i>
Between groups	7927.27	6.00	1321.21	32.30	0.00
Within groups	72732.77	1778.00	40.91		
Total	80660.04	1784.00			

Table 6 Tukey's post-hoc test for subplot scale leaf chlorophyll content measurements. Significant *I-J* mean differences are bolded. The mean difference is significant at the 0.05 level.

<i>Chlorophyll</i>					<i>95% Confidence Interval</i>	
<i>Location (I)</i>	<i>Location (J)</i>	<i>Mean Difference (I-J)</i>	<i>Std. Err.</i>	<i>Significance</i>	<i>Lower</i>	<i>Upper</i>
1	2	2.90	0.37	0.00	1.81	4.00
	3	0.02	1.12	1.00	-3.30	3.33
	4	1.41	0.56	0.15	-0.23	3.06
	5	0.86	0.92	0.97	-1.86	3.57
	6	-1.24	0.49	0.15	-2.68	0.21
	7	-5.79	0.69	0.00	-7.82	-3.77
2	1	-2.90	0.37	0.00	-4.00	-1.81
	3	-2.89	1.13	0.14	-6.23	0.45
	4	-1.49	0.58	0.13	-3.19	0.21
	5	-2.05	0.93	0.29	-4.80	0.70
	6	-4.14	0.51	0.00	-5.65	-2.63
	7	-8.70	0.70	0.00	-10.77	-6.63
3	1	-0.02	1.12	1.00	-3.33	3.30
	2	2.89	1.13	0.14	-0.45	6.23
	4	1.40	1.21	0.91	-2.16	4.96
	5	0.84	1.41	1.00	-3.33	5.00
	6	-1.25	1.18	0.94	-4.73	2.22
	7	-5.81	1.27	0.00	-9.56	-2.06
4	1	-1.41	0.56	0.15	-3.06	0.23
	2	1.49	0.58	0.13	-0.21	3.19
	3	-1.40	1.21	0.91	-4.96	2.16
	5	-0.56	1.02	1.00	-3.57	2.45
	6	-2.65	0.66	0.00	-4.60	-0.70

	7	-7.21	0.82	0.00	-9.62	-4.80
5	1	-0.86	0.92	0.97	-3.57	1.86
	2	2.05	0.93	0.29	-0.70	4.80
	3	-0.84	1.41	1.00	-5.00	3.33
	4	0.56	1.02	1.00	-2.45	3.57
	6	-2.09	0.98	0.34	-5.00	0.81
	7	-6.65	1.10	0.00	-9.88	-3.42
6	1	1.24	0.49	0.15	-0.21	2.68
	2	4.14	0.51	0.00	2.63	5.65
	3	1.25	1.18	0.94	-2.22	4.73
	4	2.65	0.66	0.00	0.70	4.60
	5	2.09	0.98	0.34	-0.81	5.00
	7	-4.56	0.77	0.00	-6.84	-2.28
7	1	5.79	0.69	0.00	3.77	7.82
	2	8.70	0.70	0.00	6.63	10.77
	3	5.81	1.27	0.00	2.06	9.56
	4	7.21	0.82	0.00	4.80	9.62
	5	6.65	1.10	0.00	3.42	9.88
	6	4.56	0.77	0.00	2.28	6.84

The descriptive statistics for the plot level leaf chlorophyll content measurements are shown in Table 7. The results of the plot level (all subplot measurements combined into one value) ANOVA (Table 8) showed that once again there were significant differences between the site means ($p > 0.05$, $F = 9.53$); however, the results of Tukey's post-hoc analysis showed that no significant differences between the destructive and instrument based chlorophyll measurements (Table 9). This result suggests that the converted SPAD values and the spectrophotometry are similar when subplot variability is removed, and that the consensus equation is acceptable for instrument conversion. It was therefore concluded that SPAD measurements, averaged to the plot level, would be appropriate for the other field sites and subsequent biochemical modelling.

Table 7 Descriptive statistics for converted SPAD values and destructive leaf chlorophyll content ($\mu\text{g}/\text{cm}^2$) for all field sites for plot level data. Plots with zero values included (some subplots had no vegetation).

<i>Chlorophyll ($\mu\text{g}/\text{cm}^2$)</i>					<i>95% Confidence Interval</i>			
<i>Site</i>	<i>n</i>	<i>Mean</i>	<i>Std. Dev.</i>	<i>Std. Err.</i>	<i>Lower</i>	<i>Upper</i>	<i>Min</i>	<i>Max</i>
1.Herschel Island 2011	33	34.9	4.5	0.8	33.3	36.5	26.8	42.6
2.Banks Island 2012	31	27.2	11.8	2.1	22.9	31.6	0.0	39.5
3.Richards Island 2012	10	37.4	4.3	1.4	34.4	40.5	31.0	45.9
4.Richards Island 2013	18	33.5	4.4	1.0	31.3	35.7	24.8	43.2
5.Tuktoyaktuk 2012	7	35.0	4.1	1.6	31.1	38.8	31.2	42.9
6.Richardson Mountains 2013	25	36.1	5.1	1.0	34.0	38.2	24.6	43.7
7.Richardson Mountains 2014	20	40.7	2.5	0.6	39.6	41.9	36.0	44.3
<i>Total</i>	33	34.9	4.5	0.8	33.3	36.5	26.8	42.6

Table 8 ANOVA results for plot level leaf chlorophyll content comparisons by field site. Results are significant at the 0.05 level.

<i>Chlorophyll</i>	<i>Sum of squares</i>	<i>Degrees of freedom</i>	<i>Mean square</i>	<i>F</i>	<i>Significance</i>
<i>Between groups</i>	2589.33	6.00	431.56	9.53	0.00
<i>Within groups</i>	6203.07	137.00	45.28		
<i>Total</i>	8792.40	143.00			

Table 9 Tukey's post-hoc test for subplot scale leaf chlorophyll content measurements. Significant *I-J* mean differences are bolded. The mean difference is significant at the 0.05 level.

<i>Chlorophyll</i>					<i>95% Confidence Interval</i>	
<i>Location (I)</i>	<i>Location (J)</i>	<i>Mean Difference (I-J)</i>	<i>Std. Err.</i>	<i>Significance</i>	<i>Lower</i>	<i>Upper</i>
1	2	7.70	1.68	0.00	2.66	12.73
	3	-2.54	2.43	0.94	-9.80	4.73
	4	1.42	1.97	0.99	-4.48	7.32
	5	-0.04	2.80	1.00	-8.42	8.34
	6	-1.23	1.78	0.99	-6.57	4.11
	7	-5.80	1.91	0.04	-11.51	-0.09
2	1	-7.70	1.68	0.00	-12.73	-2.66
	3	-10.23	2.45	0.00	-17.56	-2.91
	4	-6.28	1.99	0.03	-12.25	-0.31
	5	-7.74	2.82	0.09	-16.17	0.69
	6	-8.93	1.81	0.00	-14.34	-3.52
	7	-13.50	1.93	0.00	-19.27	-7.72
3	1	2.54	2.43	0.94	-4.73	9.80
	2	10.23	2.45	0.00	2.91	17.56
	4	3.95	2.65	0.75	-3.99	11.90
	5	2.49	3.32	0.99	-7.43	12.42
	6	1.30	2.52	1.00	-6.23	8.84
	7	-3.26	2.61	0.87	-11.06	4.53
4	1	-1.42	1.97	0.99	-7.32	4.48
	2	6.28	1.99	0.03	0.31	12.25
	3	-3.95	2.65	0.75	-11.90	3.99
	5	-1.46	3.00	1.00	-10.43	7.51
	6	-2.65	2.08	0.86	-8.87	3.58
	7	-7.22	2.19	0.02	-13.76	-0.68
5	1	0.04	2.80	1.00	-8.34	8.42
	2	7.74	2.82	0.09	-0.69	16.17
	3	-2.49	3.32	0.99	-12.42	7.43
	4	1.46	3.00	1.00	-7.51	10.43

	6	-1.19	2.88	1.00	-9.80	7.42
	7	-5.76	2.96	0.45	-14.60	3.09
6	1	1.23	1.78	0.99	-4.11	6.57
	2	8.93	1.81	0.00	3.52	14.34
	3	-1.30	2.52	1.00	-8.84	6.23
	4	2.65	2.08	0.86	-3.58	8.87
	5	1.19	2.88	1.00	-7.42	9.80
	7	-4.57	2.02	0.27	-10.61	1.47
7	1	5.80	1.91	0.04	0.09	11.51
	2	13.50	1.93	0.00	7.72	19.27
	3	3.26	2.61	0.87	-4.53	11.06
	4	7.22	2.19	0.02	0.68	13.76
	5	5.76	2.96	0.45	-3.09	14.60
	6	4.57	2.02	0.27	-1.47	10.61

3.4. Discussion and Conclusion

Arctic vegetation biochemistry was measured at the leaf and canopy scales across five field sites between the years 2011 to 2014. Field measurements taken between the years 2011 and 2013 were completed with a Minolta SPAD-502 chlorophyll meter, while measurements in the 2014 field season were completed using destructive laboratory and weighting techniques; lack of SPAD availability in 2014 did not allow for coincident measurements. The leaf chlorophyll values measured *in situ* were shown to be not significantly different from the lab-based destructive sampling methods when compared at the plot scale, indicating similarity between measurement techniques. Furthermore, a general latitudinal gradient of leaf-level chlorophyll was shown to exist with greater chlorophyll values at lower latitudes. Chlorophyll values in this study corresponded well to those of other studies (e.g. Tiezen & Johnson, 1968); however, there is an absence of studies measuring biochemicals in Arctic environments that can be used to compare against the results achieved here. Tiezen and Johnson (1968) used incorrect extinction coefficients in the wet chemical analysis and so reported pigment values were deemed erroneous. It is recommended that additional and more in-depth studies of leaf and canopy biochemistry be conducted across Arctic environments with the updated techniques of Lichtenthaler (1987) and properly calibrated handheld equipment.

A major challenge associated with sampling the average biochemical and/or biophysical attribute values associated with Arctic tundra canopies is that they are typically characterized as heterogeneous assemblages containing many species with varying leaf and canopy anatomical morphological characteristics. All species occupy what can be thought of as a micro-canopy, with heterogeneous characteristics when observed at the subplot and field scale, but as a more homogenous mixture when viewed at the remote sensing or landscape scale (e.g. medium resolution satellite imagery). Although distinct monotypic vegetation communities do exist across the Western Arctic, such as willow shrubs (e.g. teal leaf willow) that occupy gullies and wetter drainage sites, they are not the dominant plant grouping; it is more typical that vegetation assemblages are heterogeneous in nature (e.g. Laidler et al., 2008). Figure 22 shows a typical assemblage of plants viewed at the field canopy scale in the Richardson Mountains (2014). It is obvious from the photograph that leaf-based sampling is a challenging task.

Figure 22 A typical tundra canopy configuration. Photo taken in the Richardson Mountains (2014).

Whether measuring chlorophyll with destructive sampling techniques or with non-destructive handheld chlorophyll meters, there exist several methodological challenges associated with the following. (1) *Canopy heterogeneity*: Sampling design is confounded by vegetation anatomy/morphology and canopy configuration (heterogeneity). Such a problem gives rise to the following question: how can a representative measurement of chlorophyll be collected in a timely manner with a clip based chlorophyll meter when the canopy is composed of thousands of tiny leaves, many of which are not easily measurable? In this study, the averaging of leaf biochemical values (both destructive and non-destructive) across subplots was completed to account for the differing/diverging values observed at the species level. As observed in Figure 22, the vegetation types in this environment range from a few centimetres to perhaps a decimetre in height, and are a complex mix that are well distributed across the terrain. It should be noted that the selected

subplot size of 1 m² appeared to capture this distribution well at all sites. (2) *Leaf anatomy*: The anatomical/morphological characteristics of many Arctic species do not readily lend themselves to simple sampling with either spectrophotometry or clip-based chlorophyll meters, and as such varying leaf structures may confound results. For example, species such as Labrador tea have leaves much thicker than Arctic sweet coltsfoot; however, each are within the allowable leaf thickness for SPAD measurements. Furthermore, collecting a representative sample of a known surface area is very difficult with species that have extremely tiny and complex photosynthetic components (needles/leaves), such as crowberry and peat moss (and other bryophytes). Consequently, EWT measurements made on these species were also assumed to possess a degree of uncertainty (i.e. peat moss is typically saturated under natural conditions). (3) *Scaling measurements*: Translating laboratory leaf-based spectrophotometry measurements to field scale requires a prohibitively lengthy procedure that involves harvesting and sorting canopy scale plots (i.e. 1 m²) and then applying a weighting function to the sorted species using the average per-species biochemical content. Applying such weights to the sorted vegetation canopy is problematic since the average condition is used for each species (as was done in this study); however, a weighted average estimate is likely more realistic than simply using the mean of the spectrophotometric measurements over all species. Alternatively, a classification based approach (e.g. Liu et al., 2016) could be considered in future studies attempting to scale leaf level measurements to the canopy scale. (4) *Timing of measurements*: Timing of measurements is crucial since there exists a very short season for vegetation green-up (Semenchuk et al., 2016). Theoretically, all sampling should be conducted at the same time of year – a practice that is rather difficult when planning logistics in remote locations such as the Arctic. As shown in Tieszen (1972), maximal chlorophyll values for the region typically occur around July 25th. All sampling

in this research coincided with this maximal canopy development stage. Future studies should account for seasonality/phenology when characterizing the ecosystem in question as short growing seasons are typical across Arctic climates. (5) *Spatial variation*: The spatial variability of plant biochemistry may be affected by such things microclimate variability, nutrient/soil variability, sun light hours, air temperatures, moisture availability, etc. (Walker et al., 2016). These factors were not extensively considered when harvesting species for measurement.

The use of handheld chlorophyll meters, such as the SPAD used in combination with the consensus equation (Cerovic et al., 2012) is a fast and repeatable method for sampling leaf biochemistry. It is possibly a more accurate means of sampling vegetation biochemistry than wet extraction techniques, mainly because of the reproducibility of the measurements. Although the anatomical structure of the leaves can play a big role in the reliability of the consensus equation, SPAD measurements have been shown to exhibit near linear (slightly curvilinear) responses to leaf chlorophyll content across multiple environments (and species types) (Cerovic et al., 2012). Chlorophyll meters are a valuable tool for Arctic biochemical sampling because of their capacity to make many repeated measurements *in situ*, thus allowing one to avoid errors and uncertainty involved with transporting time sensitive samples. Furthermore, handheld instruments provide the benefit of non-destructively assessing intact leaves (no degradation of samples) conjointly to remote sensing image acquisitions. A problem that arises when sampling in heterogeneous canopies is deciding on an adequate number of samples to represent the average leaf condition and deciding upon a sufficiently high enough number of samples to capture the natural variability. Sampling with the SPAD in this study was tedious and time-consuming. Deciding on which leaves to sample may have introduced bias into the handheld chlorophyll measurements. Significant effort was made to ensure randomness of the samples and all leaf conditions were included, except for

completely senescent vegetation. The number of samples collected across all the plots represented a significant sample size, and certainly more than is possible using destructive techniques; such a large sample size may have eliminated any sampling biases introduced. For example, a total of 693 subplots were measured on Herschel Island, with 10 SPAD measurements per plot for a total of 6,930 SPAD measurements. To ensure that this instrument (and the consensus equation) produces accurate results in an Arctic setting, the instrument should be calibrated with wet chemical methods.

Wet chemical extraction methods are known to produce accurate results (e.g. Gitelson et al., 2009); however, there are several factors that can contribute to error or limit their usefulness. The quantitative assessment of chlorophylls ($a+b$) and carotenoids ($x+c$) using destructive spectroscopy is complicated by choice of sample (e.g. what pigment is being investigated and from what species), the organic solvent system used to extract pigments, and the spectrophotometer used (Lichtenthaler & Buschmann, 2005). Since all samples in this research were taken from intact leaves, the homogenized solutions all contained multiple pigments and therefore were complicated by overlapping absorption regions (i.e. absorption maxima) (see Lichtenthaler, 1987; Lichtenthaler & Buschmann, 2005). For example, chlorophyll *a* and *b* isolated in diethyl ether absorb in narrow bands (maxima) in the blue (near 428 and 453, respectively) and red (near 661 and 642 nm, respectively). The absorption maxima of these pigments strongly depend on the type of organic solvent used – and to some degree the spectrophotometer used (Lichtenthaler & Buschmann, 2005). If the polarity of the solvent is increased, the red absorption maximum of chlorophyll *a* will shift from 660 nm to 665 nm, and the blue absorption maximum from 428 nm to 432 nm. Chlorophyll *b* also experiences the same degree of absorption maxima shift, from 642 nm to 652 nm and 452 nm to 469 nm, respectively (Lichtenthaler, 1987). The absorption readings, therefore,

must be performed in the correct wavelength positions (maxima) for a solvent, and the solvent specific coefficients must be considered by applying the corresponding equations for the calculation of the pigment quantities (Lichtenthaler & Buschmann, 2005). In this investigation, the updated coefficients for multi-pigment assessment in 80% acetone were used (Lichtenthaler, 1987). The coefficients used before Lichtenthaler (1987) are not correct (e.g. Arnon, 1949); future studies should take this into account. Furthermore, some spectrometers differ in their wavelength positions, thus the position of maximal absorption can be shifted by 1.0 to 1.5 nm (Lichtenthaler & Buschmann, 2005). If greater than 2 nm, it is possible that the spectrophotometer needs to be adjusted or an impure solvent has been used for calibration. In this study, the spectrometer was not checked against pure solvent extracts, so its absolute accuracy was not known.

Chapter 4. Modelling Plant Area Index and Canopy Chlorophyll Content Across an Arctic Bioclimatic Gradient with Downward Hemispherical Photography

Abstract

Leaf area index (LAI, m^2/m^2), also known as plant area index (PAI, m^2/m^2) when green non-leaf plant components are included, is a main driver of canopy-scale processes and has been shown to be a useful variable in the investigation of ecosystems, climate, and retrieval of canopy scale vegetation biochemistry. In this study, the effective plant area index (PAI_e), true plant area index (PAI_t), and average leaf angle (ALA) were estimated using downward looking hemispherical photography (DHP) at all field sites. At the Richardson Mountains (2014) field site, PAI_e and PAI_t values were compared to PAI measured using a destructive method (PAI_d). The primary goal was to evaluate DHP for estimating PAI in Arctic tundra environments, specifically at multiple sites along a latitudinal gradient. The secondary goal was to provide baseline PAI values for all field sites and to provide parametrization values for subsequent physical modelling. Mean PAI values were as follows: 0.35 to 1.74 for PAI_d , 0.35 to 1.82 for PAI_e , and 0.44 to 2.00 for PAI_t . The results of DHP modelling showed strong relationships between PAI_d and PAI_e ($r^2=0.86$, $\text{RMSE}=0.15$) and between PAI_d and PAI_t ($r^2=0.77$, $\text{RMSE}=0.21$). PAI_e estimates were shown to be more accurate (closer to PAI_d values with no statistical difference between them) than PAI_t estimates and were thus used for subsequent modelling retrievals in later chapters. PAI_e values showed a north to south gradient where the lowest latitude site possessed a mean of ~ 1.14 and the highest latitude site possessed a mean of ~ 0.51 . One-way analysis of variance (ANOVA) showed that significant differences in PAI_e means existed between sites ($p \leq 0.05$). In addition, leaf chlorophyll content (LCC) measurements were scaled to the canopy level by multiplying by the PAI_e values

to obtain the effective canopy chlorophyll content (CCC_e). One-way ANOVA showed that there were also statistically significant differences in CCC_e values between field sites ($p \leq 0.05$).

4.1. Introduction

Leaf area index (LAI, unitless [m^2/m^2]), measured as the ratio of total upper leaf surface area divided by the surface area of the land over which the vegetation grows, is a key plant characteristic within ecological research and monitoring (Watson, 1947; Boelman et al., 2003, Breda 2003, Ewert 2004, Van Wijk et al., 2005; Mougin et al., 2014). LAI has been linked to atmosphere-vegetation exchange processes, such as photosynthesis, evapotranspiration, and carbon flux (Soegaard, 1999; Leuning et al., 2005; Duchemin, et al., 2006; Cleugh et al., 2007; Jongschaap, 2006; Chen et al., 2006; Chen et al., 2007; Zheng & Moskal, 2009). Quantitative estimates of LAI can provide an understanding of dynamic changes in ecosystem productivity and offer a metric for which climate related impacts on ecosystems can be assessed (Zheng & Moskal, 2009). Remotely-sensed measurements of LAI are therefore an important component to monitoring and modelling of ecological variables and processes both spatially and temporally (Green et al., 1997; Liu et al., 1997; Zheng & Moskal, 2009). Additionally, LAI is a necessary parameter/variable used in leaf-canopy radiative transfer models (RTMs) such as PROSAIL (Jacquemoud et al., 2009) and can further provide a means for scaling leaf-level biochemical variables to the canopy level (Darvishzadeh et al., 2008a,b, Croft et al., 2014; Verrelst et al., 2015b; Peng et al., 2017; Clevers et al., 2017). Green and woody non-leaf components, the latter being less common in Arctic tundra vegetation, are typically included in the characterization of low canopies. Although the literature refers mostly to LAI, the term used in this study and in some papers using indirect estimation methods is plant area index (PAI, m^2/m^2) (Neumann et al., 1989; Jonckheere et al., 2004). In this

study, only green, non-woody vegetation components were considered in the estimation of PAI (Mougin et al., 2014).

Another important canopy parameter/variable is the leaf inclination distribution function, which refers to the angular orientation of the leaves in the vegetation canopy; specifically, their zenith and azimuth angles (Wang et al., 2007). It is typically referred to as leaf angle distribution (LAD), and when averaged, as the average leaf angle (ALA, hereafter). ALA is a key variable that has been shown to play a role in energy and mass balance in atmosphere-vegetation exchange processes including micro-climate processes (Thanisawanyangkura et al., 1997; Wang et al., 2007). ALA can be extremely variable between species within a plant canopy and between different canopy areas (Jane et al., 2001) and because of this exhibits a high degree of spatial and temporal variability (Wirth et al., 2001). Few approaches have been proposed to estimate ALA from optical and remotely-sensed data (Jonckheere et al., 2004; Weiss et al., 2004; Casa & Jones, 2005; Damarez et al., 2008; Mougin et al., 2014). ALA is a common parameter/variable in canopy RTMs, such as PROSAIL (Jacquemoud et al., 2009).

Many destructive and non-destructive methods have been developed to quantify LAI and ALA, both directly and indirectly at the field scale (Breda, 2003; Jonckheere et al., 2004; Weiss et al., 2004). Accurate quantification of both LAI and ALA remains difficult due to the large spatial and temporal variability of vegetation canopies (Breda, 2003). Measuring LAI in low canopy Arctic environments, for example, can pose a significant challenge due to the morphological nature of the vegetation species (e.g. mosses, lichens, needles vs. broad leaves, grasses, etc.) and the physiological configuration of the canopy (i.e. low-lying stature; high vegetation density) (Van Wijk et al., 2005; Williams et al., 2008; Chen et al., 2009). Direct destructive methods for estimating *in situ* LAI are time and labour intensive and difficult to implement over large areas

and numerous sample sizes (Jonckheere et al., 2004; Weiss et al., 2004). Indirect, non-destructive methods that use optical sensors are therefore recommended for extensive ground sampling since they are relatively simple to utilize (Mougin et al., 2014). Sensors such as the LAI-2000 Plant Canopy Analyzer (Welles, 1990) or TRAC (Tracing Radiation and Architecture of Canopies) (Leblanc et al., 2002) estimate LAI from light transmittance measurements, while others such as hemispherical photography (Frazer et al., 2001) provide canopy gap fraction from image analysis (Demarez et al., 2008). Digital hemispherical photography (DHP) used in combination with classification software, such as CAN-EYE (Weiss et al., 2004, Weiss & Baret, 2016), which was used in this research, is now a common and efficient technique for monitoring LAI/PAI in low/sparse canopies (e.g. Demarez et al., 2008; Mougin et al., 2014).

The model normally used to determine LAI from indirect methods (e.g. DHP) is the Poisson law (Demarez et al., 2008). The Poisson law assumes that all leaves within a canopy are uniformly and randomly distributed (Demarez et al., 2008). This is a sound assumption for homogenous canopies (Levy & Jarvis, 1999), but is not correct for canopies with patterns and clumping properties, such as row crops or forests (Baldocchi & Collineau, 1994; Demarez et al., 2008). For canopies with patterns, the effective LAI (LAI_e) has been proposed (e.g. Chen, 1996b) and allows for the use/incorporation of the Poisson law; LAI_e corresponds to the product of a clumping index with the true LAI estimate (Chen & Cihlar, 1995a; Demarez et al., 2008). CAN-EYE provides estimates of LAI_e using the Poisson law, as well as several other parameter/variable estimates such as true LAI (LAI_t), and the cover fraction (f_{Cover}) (Demarez et al., 2008). CAN-EYE classifies DHP images interactively in red/green/blue colour space, which differs from simple image thresholding procedures that are applied using an index or monochromatic colour. Additionally,

the software allows for bulk processing of DHPs, a feature that allows for the capture of canopy spatial variability (Demarez et al., 2008).

Studies that have quantified the spatial variability of LAI in Arctic environments (low canopies with heterogeneous configurations) using various ground techniques are numerous (e.g. Walker et al., 2003; Laidler et al., 2008; Walker et al., 2012). However, no studies have examined the use of DHP for LAI retrievals in Arctic environments. Campioli et al., (2009) investigated the use of photography for estimation of LAI from harvested vegetation in sub-Arctic (Sweden) and high Arctic (Greenland and Svalbard) sites; however, this study did not use DHP for *in situ* LAI estimation. Previous studies using DHP to measure LAI in other short canopy environments have reported and demonstrated its effectiveness for fast, simple, and accurate retrievals of LAI (e.g. Demarez et al., 2008; Mougin et al., 2014). Therefore, the use of DHP presented itself as a potentially viable means of retrieving canopy structural variables, such as LAI and ALA, in the Arctic environments of this study.

Considering the above, the primary objective of this study was to determine if non-destructive DHP modelling could provide useful predictions of LAI (hereafter referred to as PAI) across heterogeneous Arctic tundra environments. The second objective was to determine which of the DHP modelling outputs, effective plant area index (PAI_e) or true plant area index (PAI_t) (following CAN-EYE terminology), were a better predictor of destructive measurements of plant area index (PAI_d) (a field-based destructive method). The third objective was to measure PAI using DHP across a latitudinal gradient in the Western Canadian Arctic to determine if there was a statistically significant difference between low latitude values and high latitude values. Following this, previously measured leaf chlorophyll content (LCC) values (Chapter 3) were scaled to canopy chlorophyll content (CCC) and assessed for statistically significant latitudinal differences.

Measurements were carried out in multiple seasons, with each sampling period being at the height of the growing season to capture maximum canopy development. The fourth objective of the PAI modelling was to provide calibration, validation, and parameterization values for subsequent empirical and physical modelling efforts, including estimates of ALA.

4.2. Materials and Methods

4.2.1. Field sites

From the study areas described in Chapter 2, one was selected as a representative example of heterogeneous tundra vegetation assemblages. Non-destructive DHP and concomitant destructive field sampling was conducted between July 20th and August 5th, 2014 in the Richardson Mountains along the Dempster Highway on the border between the Yukon Territory (YT) and Northwest Territories (NT). A map of the study area and locations of the destructively sampled ground plots can be seen in Figure 10 (Section 2.1.4.).

Non-destructive DHP PAI measurements had been previously taken at all the study areas on the following dates: (1) July 18th to July 29th, 2011 Herschel Island, YT; (2) July 10th to July 20th, 2012 on Banks Island, NT; (3) July 25-26th, 2012 Richards Island, NT, (4) July 24th, 2012 Tuktoyaktuk, NT, 2012, (5) July 25th to August 4th, 2013 on Richards Island, NT, and (6) July 18th to July 22nd, 2013 in the Richardson Mountains, YT/NT.

As for the chlorophyll field sampling and lab measurement (Chapter 3), the Richardson Mountains field site was chosen for destructive sampling due to its accessibility by road and its proximity to ARI. All other field sites were in remote locations where destructive sampling was not practical (e.g. Banks Island), and as such, *in situ* DHP measurement was considered the best option in these locations.

4.2.2. Destructive LAI measurements

The field site was first divided into distinctive vegetated landscape zones using a stratified sampling approach to establish potential plot locations. Spectrally distinct areas were identified through visual analysis of Landsat 5 and 8 imagery and through on-the-ground identification of distinctly different vegetated areas using car surveys and by climbing mountains. Within these vegetation zones, field plot locations were randomly selected. Twenty plots measuring 90 m x 90 m were selected within homogenously vegetated areas away from borders and transitional zones. Each plot was systematically sampled using three equally spaced transects. The three transects were subdivided into seven 1 m² subplots that were used for non-destructive DHP measurements (Figure 23), while five of the 1 m² plots were systematically chosen for destructive measurements (shown in red, Figure 23). The central location of each square was recorded using a Trimble Juno handheld GPS unit (accurate to approximately ~3 m).

Sampling Strategy Herschel Island shown

Figure 23 Diagram showing the destructive PAI (red squares) and non-destructive DHP sampling (white/red squares) strategies. Herschel Island shown as an example.

All leafy vegetation and associated green stems were clipped within each of the 1 m² plots, bagged, and placed in a cooler to prevent degradation. Figure 24 (left) shows the harvesting of vegetation at a typical subplot. Sphagnum was not included in the samples unless dominant and visibly exposed – only the top green components were clipped if present (i.e. the green components visible to the camera). Lichen was not included in any of the samples. A total of 99 subplots were harvested across the 20 plots (one subplot was discarded). Samples were transported to the lab and processed the same day.

Figure 24 Collecting canopy samples at the subplot scale (1 m²) (left). Example of the setup used to photograph the destructive PAI canopy samples (right).

Figure 24 (right) shows the method in which PAI was measured destructively. All samples were laid out on a white sheet measuring 180 cm by 180 cm to minimize the amount of leaf/stem overlap. They were then photographed with a Nikon D300 SLR camera equipped with the same hemispherical lens used for the DHP sampling as described in Section 4.2.7 (Sigma 8mm F3.5 EX DG Circular Fisheye, Sigma Corp., Bandai, Fukushima, Japan). Green and mostly green vegetation was kept for the analysis (corresponding to the condition of the vegetation sampled for biochemistry); completely senescent non-photosynthetic vegetation was discarded, given the DHP image processing method described in Section 4.3.2 below is based on a classification of green vegetation. All images were photographed from a constant height of 1.5 m, corrected for lens distortion using Photoshop CS6 (Camera Raw), and then cropped/resized to 1800 x 1800 pixels (total pixels = 3,240,000) so that each pixel represented 0.1 cm in both the x and y directions (area = 0.01 cm²). Once each image was corrected for lens effects/distortion and cropped, a thresholding filter was applied that converts a colour image into a high contrast black and white binary image using a user-specified threshold (selected through analysis of the image histogram). All pixels

brighter than the threshold were converted to white; and other pixels were converted to black. Since only green vegetation components were considered, thresholding was completed on green colours. All thresholding was completed with Adobe Photoshop CS6 (Adobe Inc.). Figure 25 shows a corrected image with its binarized result. Once thresholding was applied to an image, the total number of black pixels was divided by the image total (i.e. 3,240,000) to obtain the PAI_d (or the known pixel area in cm^2 was divided by the area of the subplot in cm^2). All measured subplots (e.g. $n=5$) belonging to each plot ($n=20$) were averaged to produce one PAI_d value for each of the five positions along the transect, amounting to a total PAI_d sample size of 20. Image thresholding proved to be a more rapid and accurate method than classifying images with traditional remote sensing software using unsupervised techniques (e.g. ISODATA and k -means).

Figure 25 Corrected (left) and binarized image (right) of destructive plant area index (PAI_d) measurements.

4.2.3. CAN-EYE and Downward Hemispherical Photography (DHP)

The CAN-EYE software provides estimates of the effective (PAI_e) and estimates of the true PAI (PAI_t) through an adjustment of the clumping index (Weiss et al., 2004, Demarez et al., 2008;

Weiss & Baret, 2016) that is based on the Lang and Yueqin (1986) averaging method (Demarez et al., 2008). The main outputs of the software when using DHP inputs are plant area index (PAI), average leaf inclination angle (ALA), fraction of absorbed photosynthetically active radiation (f APAR) (not discussed in this thesis, as poor relationships with chlorophyll were observed), the vegetation cover fraction (f Cover), the bidirectional and mono-directional gap fraction, and clumping index. Note that only f Cover is output using a normal lens pointed vertically downward. With a normal lens pointed at 57° PAI can be derived. However, in this research, to derive all of the above parameters, particularly PAI and ALA, which are important parameters in the physically-based modelling of Chapters 6 and 7 (and Chapter 2.2.3 – background), a hemispherical lens was required. Before using the CAN-EYE software with the desired camera and lens combination, a calibration procedure must be completed as per Weiss & Baret (2016) (described in Section 6, “DHP Calibration Module”, of the CAN-EYE V6.4.6 manual).

The CAN-EYE software is capable of processing multiple images at once, a feature that speeds up processing time considerably over one-at-a-time methods (up to 25 images can be processed at once, with a minimum of 8) (Wiess et al., 2004). For each set of DHPs (e.g. 21 per plot in this research) gap fraction was calculated through supervised classification to produce one set of modelled outputs. The original 16,777,216 image colours are reduced to 327 using an automatic classification (Spath, 1985). CAN-EYE classifies mixed pixels as one of the two classes based on their position within the colour space (Demarez et al., 2008). All pixels contaminated with undesirable objects (e.g. people) were masked. Each classification attempt was then refined interactively to produce the most visually appealing result (i.e. green vegetation was properly classified). Finally, in accordance with Damarez et al. (2008) the DHP classification process was completed using the vegetation-based classification, since it was shown that soil-based

classification can lead to an underestimation of gap fractions (i.e. shadows are erroneously classified as leaves). For this research, the software was set to automatically classify pixels that were not vegetation as gaps (e.g. soil and other background).

4.2.4. Effective PAI estimation based on gap fraction

Image classification was done in angular sectors with a zenith ($\Delta\theta$) resolution equal to 2.5° and an azimuth ($\Delta\varphi$) resolution equal to 2.5° . Demarez et al. (2008) have stated that there is little sensitivity of PAI_e estimates to changes in the zenith and azimuth resolution and so the highest resolution was used for the analysis. After images were classified, the gap fraction ($P_{o,CAN-EYE}(\theta)$) was computed for each zenithal ring by taking the average values for all inputted photographs across the 72 azimuthal sectors, excluding the masked areas. For DHP, gap fraction estimates are based on the transmittance of light through the canopy; the absorbing green vegetation elements are considered opaque/black (Zhao et al., 2012; Mougin et al., 2014). PAI_e is computed from the gap fraction using the Poisson law (distribution) as in Equation 11 (Welles & Norman, 1991; Demarez et al., 2008):

$$P_{o,CAN-EYE}(\theta) = \frac{\exp\left(-PAI_e * G(\theta, \varphi, \theta_{leaf,eff})\right)}{\cos \theta} \quad (11)$$

where θ and φ are the zenith and azimuth angles of the direction of propagation of the incident beam, PAI_e is effective PAI , and $G(\theta, \varphi)$ is the mean projection of leaf area onto a plane perpendicular to direction (θ, φ) which is directly dependent on the leaf angle distribution (LAD) (Demarez et al., 2008). LAD is considered uniform in azimuth and ellipsoidal in inclination distribution; LAD is characterized with the average leaf angle (ALA) (Campbell, 1986; Wang & Jarvis, 1988; Demarez et al., 2008). Canopy architecture is therefore fully characterized/described by two parameters when being estimated with the inclusion of the gap fraction (for which the two

terms adopt the “effective” descriptor): the effective PAI and the effective ALA ($\theta_{leaf,eff}$). A look-up-table (LUT) provides the means for estimating PAI_e and ALA_e from the measured zenithal variation of the gap fraction (Weiss et al., 2004). The LUT was computed through random combinations of PAI_e values between 0 and 10, using increments of 0.01, and ALA_e values between 10° and 80° , using increments of 2° (Demarez et al., 2008). Equation 12 shows the cost function J , representing the distance between measured and estimated gap fractions evaluated over the 36,036 PAI_e and ALA_e pairs:

$$J = \sqrt{\sum_{\theta} \left(\frac{P_{o,LUT}(\theta_i, PAI_e, \theta_{leaf,eff}) - P_{o,CAN-EYE}(\theta_i)}{\sigma_{P_{o,CAN-EYE}}} \right)^2 + \left(\frac{\theta_{leaf,eff} - 60}{30} \right)^2} \quad (12)$$

where $P_{o,CAN-EYE}(\theta_i)$ is the measured gap fraction derived from CAN-EYE, $P_{o,LUT}(\theta_i, PAI_e, \theta_{leaf,eff})$ is the gap fraction stored in the LUT, and $\sigma_{P_{o,CAN-EYE}}$ is the standard deviation of the CAN-EYE measured gap fraction (Weiss et al., 2004; Demarez et al., 2008). The secondary term in equation 2 imposes constraints on the retrieved ALA_e values and regularizes the ill-posed nature of the inversion (Combal et al., 2002). The solution to the inversion is the PAI_e and ALA_e values that minimize the cost function J . PAI_e values were compared to PAI_d values using the coefficient of determination (r^2) and root mean square error (RMSE). It should be noted that PAI_d values are not considered as an absolute reference, and as such, all RMSE calculations (i.e. PAI_e and PAI_t) are in relation to these PAI_d estimates.

4.2.5. True PAI and ALA estimates

PAI_t was calculated using the Lang and Yueqin (1986) method of averaging gap fractions (i.e. the clumping index), which assumes phytomass elements are randomly distributed in the canopy (Demarez et al., 2008). Each zenithal ring is divided into cells of 2.5° in zenith and 4° in azimuth.

The gap fraction $P_{o,cell}(\theta)$ is computed for each cell following the modified Poisson law (Equation 13):

$$P_{o,cell}(\theta) = \frac{\exp\left(-\lambda_{LX}(\theta, \theta_{leaf,eff}) * L_{LX}G(\theta, \varphi, \theta_{leaf,LX})\right)}{\cos \theta} \quad (13)$$

The gap fraction $P_{o,cell}(\theta)$ is averaged over azimuth and zenith rings for each photograph. The clumping index $\lambda_{LX}(\theta, \theta_{leaf,eff}, P_{o,cell})$ is defined as (Equation 14):

$$\lambda_{LX}(\theta, \theta_{leaf,eff}) = \frac{\text{mean}\left(\log\left(P_{o,cell}(\theta)\right)\right)}{\log\left(\text{mean}\left(P_{o,cell}(\theta)\right)\right)} \quad (14)$$

The algorithm then proceeds in the same manner as previously described for PAI_e creating an LUT for PAI_t, ALA_t, and the corresponding clumping index using the modified Poisson law. The clumping index (Chen & Black, 1992; Chen et al., 2005) provides valuable information on the spatial and temporal heterogeneity of vegetation cover (Pisek et al., 2013; Mougin et al., 2014) and is an important factor in the calculation of PAI_t (Chen et al., 2005; Zhao et al., 2012). Since leaves and needles are not normally randomly distributed in canopies (i.e. foliage exhibits different degrees of organization with different plant structures/morphologies), actual light penetration will deviate from the theoretical model of negative exponential attenuation with depth (e.g. Beer-Lambert Law) as a function of increasing PAI (Zhao et al., 2012). In Arctic ecosystems, and most vegetated ecosystems in general (e.g. forests) clumping occurs at several spatial scales: at the leaf/needle scale where photosynthetic elements are clustered around branches/stalks, at the canopy scale where leaf/branch elements are clustered around individual plants, and at the landscape scale where individual plants form the canopy. These clumping effects also vary by species. As for PAI_e, modelled PAI_t values were compared to PAI_d values using the r^2 and RMSE.

4.2.6. Estimation of $fCover$

The vegetation cover fraction ($fCover$) is the fraction of ground surface covered by green vegetation (Weiss et al., 2004; Mougin et al., 2014). To correctly measure $fCover$, photographs must be taken at nadir position (Korhonen et al., 2006). $fCover$ represents all areas not classified as gaps in the direction $\theta = 0$ (Equation 15):

$$fCover = 1 - P_o(0) \quad (15)$$

It should be noted that the gap fraction cannot be obtained exactly at nadir using DHP since only one pixel exactly corresponds to this direction; however, if the angle is narrow the bias is not significant (Bonnor, 1967; Mougin et al., 2014). CAN-EYE can integrate gap fraction estimates over a range of zenith angles (0° to 10°) to determine $fCover$; 10° was used for all sites in this research. Finally, $fCover$ values were compared to PAI_d values as for the other metrics described above.

4.2.7. Downward Hemispherical Photography (DHP)

Downward looking hemispherical photographs were taken in raw format at the highest possible resolution (4288 x 2848) with a Nikon D300 SLR camera (Nikon Corp., Tokyo, Japan) equipped with a hemispherical lens (Sigma 8 mm F3.5 EX DG Circular Fisheye, Sigma Corp., Bandai, Fukushima, Japan). The camera was set to aperture priority with an f -stop of 5.6.

Downward hemispherical photographs were taken at each plot/subplot in accordance with the sampling scheme in Figure 23. At each plot, a total of 21 subplot photographs were taken across the three transects (red and white squares in Figure 23), each from an approximate height of 1.5 m. Twenty-one photographs per plot was considered an acceptable sample size to capture canopy spatial variability (Weiss et al., 2004; Demarez et al., 2008; Mougan et al., 2014; Weis & Baret,

2016). To save time photographs were taken by hand (e.g. outstretched arm at standing position) approximately perpendicular to the ground. Sensitivity analyses has demonstrated that an uncertainty of about 10° is acceptable using CAN-EYE (Demarez et al., 2008). Due to the limited time for this remote fieldwork, photographs were taken at all sky conditions and times of day. Figure 26 shows the position of the camera for various ground plots. All photos were batch processed in Photoshop to correct white balance and exposure, and to partially eliminate shadowing, which varied between photos depending on sky conditions. After correction, images were converted to the highest quality JPEG using the same image resolution.

Figure 26 Various canopy configurations measured in the Richardson Mountains (2014) using downward hemispherical photography (DHP). Clockwise from top left: field plots 2, 7, 16, and 17.

For all series of photographs, the processing was limited to view zenith angles (VZA) equal to and less than 45° to limit the number of mixed pixels (at greater view angles) and limiting the field

of view to be just larger than the subplot (i.e. 1 m²) from which the destructive measurements would be subsequently taken. Because the Nikon D300 uses a DX-format sensor (cropped sensor) and the Sigma lens is intended for use with a FX-format sensor (full frame sensor), raw DHP photographs appear cut-off on the top and bottom (Figure 26). The use of a 45° circle of interest (COI) provided the necessary plot coverage while eliminating the cropped image portions and also allowing for the estimation of $fCover$ at 10° (as stated previously).

Finally, effective canopy chlorophyll content (CCC_e , g/m²) values were calculated by multiplying leaf chlorophyll content measurements ($\mu\text{g}/\text{cm}^2$) (see Chapter 3) by PAI_e values (found to be a better measure of PAI than PAI_t as described below). CCC_e has been used in other studies as a means of scaling up leaf-scale measurements and assessing canopy level chlorophyll content (Blackburn et al., 1998a,b; Gitelson et al., 2005; Yin et al., 2016; Croft et al., 2014; Verrelst et al., 2015b; Peng et al., 2017; Clevers et al., 2017). It provides a more useful predictor of CCC than simply using LCC since the spatial extent of vegetation cover is considered in the scaling. CCC_e values were assessed over the full set of field sites using analysis of variance (ANOVA). Subgroup means were explored through Tukey's post-hoc analysis.

4.3. Results

The following results are presented: (1) descriptions of canopy spatial variability, measured and modelled clumping and gap fractions, and visual assessment of DHP classification accuracy; (2) PAI_d values compared to PAI_e , PAI_t , and $fCover$ estimates; (3) the statistical comparison of DHP derived PAI_e and ALA_e values between field sites along a latitudinal gradient; and (4) the statistical comparison of CCC between field sites along a latitudinal gradient. All results are for the Richardson Mountains (2014) field season except for the last section which shows the results based on DHP sampling over all field sites (2011-2014).

4.3.1. Spatial variability: Gap fraction and clumping index

Analysis of the 2014 Richardson Mountains DHPs showed that vegetation canopies possessed a wide variety of configurations and a high degree of spatial variability, observations that are consistent with other Arctic studies measuring leaf area (e.g. Laidler et al., 2008; Walker et al., 2012; Liu et al., 2017). Figure 27 shows example photos cropped to 45° (top) and their corresponding vegetation-soil classifications (bottom two rows). It is evident that DHP is capable of effectively classifying green and non-green components within a scene; however, some over-estimation of green components was difficult to avoid, as can be seen in the bottom centre classified image, even when classifications were interactively performed to achieve best results. DHPs were taken during varying sky conditions, with some images acquired during full sun; however, misclassifications in low lying canopies like this were mostly due to pixel colour similarities and not shadowing. Demarez et al. (2008) have stated the importance of camera configuration and illumination condition when sampling, and have stated that downward configuration in theory allows for a wider spatial representation but can also lead to poor gap fraction estimates under sunny illumination conditions (where shadowing is intense). In this study, locations with taller canopies and hummocky terrain, derived gap fractions and clumping increased with increasing sun zenith angle under sunny conditions due to the higher prevalence of shadow. DHPs with high proportions of shadow were discarded from the analysis when shadows could not be effectively removed with image processing. Similar to the sampling of agricultural crops with DHPs (Demarez et al., 2008), overcast conditions are preferred when sampling Arctic tundra canopies, but this is not always feasible in remote regions and when fieldwork needs to be completed in a timely manner.

Figure 27 Top two rows: original DHP images. Bottom two rows: corresponding CAN-EYE classified images with vegetation (green) and soil/non-vegetation (brown). Masked areas are in black. Photos are from plot 16 (top row of each) and plot 17 (bottom row of each).

The spatial variability of vegetation and canopy configuration in the Arctic is due to numerous factors, such as thermal processes (e.g. permafrost, freeze thaw cycles, and resultant patterned ground), water and nutrient availability, plant growth characteristics, and microclimate/climate variability (e.g. sunlight and slopes) (Walker et al., 2016; Liu et al., 2017). In general, wetter sites showed thicker/greener canopies that possessed lower gap fractions and less clumping (i.e. more uniform distribution of vegetation elements), whereas drier sites had larger gap fraction and more vegetation clumping due to the prevalence of soil and rock background (gaps) and the types of

species that grow in these conditions (clumping). In most DHPs, a decrease in gap fraction with increasing VZA (i.e. further from nadir) was noted and was likely due to an increasing spatial representativeness of the pixels where soil and vegetation components were more likely to be mixed (i.e. mixed pixels). However, because a 45° COI was utilized (and photos were taken at a height of 1.5 m), gap fractions within the 0° to 45° VZA field of view that might be the result of mixed pixels and larger spatial representations, was expected to be minimized as compared to using VZAs greater than 45° (i.e. a larger COI). Figure 28 shows a variety of gap fractions for low to high $PAI_d/PAI_e/PAI_t$ values. As stated above, an overall decrease in gap fraction with increasing VZA is evident; however, this is not always the case as can be seen in Figure 28 (bottom right). Such gap fractions may be simply attributable to the high spatial variability of canopy configurations and sampling design. The gap fraction values derived from both the Poisson law (PAI_e) and modified Poisson law (PAI_t) are in general agreement with measured values derived from the DHP image classifications (Figure 28) and modelled values are very much in agreement with each other. However, the relationship between VZA and gap fraction was observed to be poorer for lower PAI values (Figure 28, bottom). The high degree of variability in estimated gap fraction between photos is evidence of the high degree of spatial variability in vegetation type and cover encountered at this site and this was similar to DHP results in all the other field sites.

Figure 28 Canopy gap fraction vs. view zenith angle (VZA) for various canopy configurations across the Richardson Mountains (2014) study site. Field plots 2, 7, 16, and 17 (clockwise from top left) are shown. Graphs show modelled (Poisson law and modified Poisson law) gap fractions for effective PAI (PAI_e) and true PAI (PAI_t) as well as gap fraction measured from the classified DHP images.

The clumping index for various canopy configurations sampled in the Richardson Mountains can be seen in Figure 29. Clumping estimates correspond to the PAI_t estimates (modified Poisson law); however, PAI_e and PAI_t values are indicated within Figure 29.

Figure 29 Clumping index vs. view zenith angle (VZA). Field plots 2, 7, 16, and 17 are shown (clockwise from the top left). Measured clumping index values were obtained through zenithal variation of gap fractions within the DHPs whereas modelled values are determined through the inversion of the modified Poisson law LUT.

For all plots in the study area, measured clumping values ranged from approximately 0.77 to 0.93 with a mean value of 0.88 and modelled clumping values of 0.77 to 0.93 with a mean value of 0.88, indicating a small degree of aggregation of leaf/vegetation elements. The values reported here are higher than those reported by Demarez et al. (2008) for agricultural crops (corn), but more in line with those reported by Mougin et al. (2014), where mean clumping index values of 0.84 are

reported for a Sahelian herbaceous canopy – an environment with short sparse canopies (however, they reported LAI values of 0.01 to as high as 5.0). The overall average gap fraction and clumping index for all sample plots can be seen in Figure 30 (left). The averaged gap fractions were generally low as many plots had continuous sphagnum ground cover, and this reduces the overall gap fraction to those seen in Figure 30 (right). Also, not surprisingly, average gap fraction decreased slightly across all plots with increasing VZAs. Clumping index remained consistent across all sites and showed slight decreases with increasing VZAs.

Figure 30 Mean clumping index and mean gap fraction for view zenith angles (VZA) of 0-45° (Richardson Mountains (2014) study area).

4.3.2. Comparison between PAI_d and modelled PAI_e , PAI_t , and $fCover$

Destructive PAI (PAI_d) values were strongly correlated with both DHP estimates of PAI_e ($r^2=0.86$, $RMSE=0.15$) and PAI_t ($r^2=0.77$, $RMSE=0.21$); Figure 31 shows these two relationships. The percent relative error (RE) values for PAI_e (RE=12.8%) and PAI_t (RE=14.3%), relative to PAI_d , were considered acceptable. Overall, RE values of <15% were deemed to be good. PAI_e values did not suffer greatly from the systematic skew that leads to the well-known

underestimation of PAI_e in clumped canopies (Demarez et al., 2008); furthermore, the use of the modified Poisson law (PAI_t) did not produce better estimates of PAI_d than the regular Poisson Law. This contrasts with a study conducted by Demarez et al. (2008) where PAI values appeared to improve globally using the modified Poisson law. However, DHP modelled values of PAI_t were higher overall than PAI_e (and resulted in greater RMSE when compared to reference PAI_d values). Since these investigations took place at peak season, it is not known if the same PAI_e and PAI_t relationships would hold over the course of the growing season. Table 10 shows all the modelled DHP outputs for the Richardson Mountains (2014) field site. Since the PAI_e results showed a stronger relationship to PAI_d and had a smaller RMSE, a decision was made to use PAI_e in all subsequent empirical and physical modelling efforts.

Figure 31 Destructive PAI (PAI_d) vs. effective PAI (PAI_e) (left) and PAI_d vs. true PAI (PAI_t) (right).

f Cover derived from the modelled gap fraction was moderately correlated with PAI_d ($r^2=0.58$), while the percent cover determined from the DHP image classification proportions for vegetation and soil had a stronger relationship ($r^2=0.77$; the relationship for vegetation is the inverse of that for soil) (Figure 32).

Figure 32 f Cover derived from DHP-modelled gap fraction vs. destructive plant area index (PAI_d) (left). Soil and vegetation percent cover derived from DHP image classification vs. destructive plant area index (PAI_d) (right).

Finally, the mean ALA_e value produced from the PAI_e model outputs ranged from 20.6° to 66.4° with an overall mean of 45.9° . There was no relationship between PAI_e and ALA_e ($r^2=0.00$). The mean ALA_e value produced from the PAI_t model output ranged from 10.0° to 70.0° with a mean of 37.0° . Similarly, there was also no relationship between PAI_t and ALA_e ($r^2=0.03$). Like the choice to retain PAI_e for the remaining modelling analyses in subsequent chapters, the corresponding effective ALA values were also retained.

Table 10 CAN-EYE modelled results and their associated r^2 , RMSE, and percent relative error (RE).

<i>CAN-EYE Variable</i>	<i>~Mean</i>	<i>~Min/Max</i>	<i>Std. Dev.</i>	<i>r²</i>	<i>RMSE</i>	<i>RE (%)</i>
<i>Measured (n=99)</i>	<i>1.18</i>	<i>0.35 / 1.74</i>	<i>0.40</i>	-	-	-
Effective PAI (n=20)	1.14	0.35 / 1.82	0.42	0.86	0.15	12.78
True PAI	1.20	0.44 / 2.00	0.45	0.77	0.21	14.30
f Cover	0.50	0.16 / 0.71	0.15	0.58	-	-
Classified Vegetation (%)	51.91	19.51 / 70.54	14.44	0.79	-	-
Classified Soil (%)	48.09	29.46/80.49	14.44	0.79	-	-
Effective ALA ($^\circ$)	45.92	20.60/66.40	13.20	0.00	-	-
True ALA ($^\circ$)	37.00	10.00/70.00	21.70	0.03	-	-

4.3.3. Comparison of modelled CAN-EYE PAI_e , and ALA_e values between sites

When all site modelled PAI_e values are plotted using standard box and whisker plots (Figure 33, left), it is evident that PAI_e generally decreases with increasing latitude as observed in similar studies (Walker et al., 2003). A latitudinal gradient was also observed for canopy gap fraction values derived both from DHP modelling and soil/vegetation classification (Figure 33, right). Quantification of such gap fraction gradients has not been previously reported for Arctic environments.

Figure 33 Modelled PAI_e values vs. latitude of the field sites (left). Gap fraction derived from DHP modelling and measured from classified DHP images vs. latitude (right). PAI_d derived values denoted with *. The boxplot shows the interquartile range with factor of 1.5; outliers are displayed with a +.

Descriptive statistics for all PAI_e values can be found in Table 11. Table 12 presents the one-tailed (ANOVA) results for PAI_e and field site (latitude gradient) showing that site PAI_e means were statistically significantly different from one another ($p \leq 0.05$, $F=17.97$). Subgroup means

compared using a Tukey's post-hoc analysis (Table 13) showed that PAI_d measurements and CAN-EYE modelled PAI_e for Richardson Mountains (2014) were not significantly different ($p \geq 0.05$), thus giving indication that the CAN-EYE estimates are a good representation of measured PAI_d values. It was also found that the Richardson Mountains 2013/2014 PAI_e values were not statistically different from one another.

Table 11 Descriptive statistics for plot level PAI_e values for all field sites. PAI_d derived values denoted with *.

<i>Effective PAI (PAI_e)</i>					<i>95% Confidence Interval</i>			
<i>Site</i>	<i>n</i>	<i>Mean</i>	<i>Std. Dev.</i>	<i>Std. Err.</i>	<i>Lower</i>	<i>Upper</i>	<i>Min</i>	<i>Max</i>
1.Herschel Island 2011	33	0.82	0.26	0.04	0.72	0.91	0.50	1.40
2.Banks Island 2012	31	0.44	0.27	0.05	0.35	0.54	0.00	0.98
3.Richards Island 2012	10	0.60	0.22	0.07	0.44	0.75	0.30	0.95
4.Richards Island 2013	18	0.80	0.25	0.06	0.68	0.92	0.34	1.43
5.Tuktoyaktuk 2012	7	0.73	0.34	0.13	0.41	1.04	0.34	1.38
6.Richardson Mountains 2013	25	1.09	0.22	0.04	0.99	1.18	0.61	1.50
7.Richardson Mountains 2014	20	1.14	0.42	0.09	0.94	1.33	0.35	1.82
8.Richardson Mountains 2014*	20	1.18	0.40	0.09	1.00	1.37	0.35	1.74
<i>Total</i>	164	0.85	0.39	0.03	0.79	0.91	0.00	1.82

Table 12 ANOVA results for PAI_e comparisons by field site at the plot scale.

<i>PAI_e</i>	<i>Sum of squares</i>	<i>Degrees of freedom</i>	<i>Mean square</i>	<i>F</i>	<i>Significance</i>
<i>Between groups</i>	11.21	7.00	1.60	17.97	0.00
<i>Within groups</i>	13.90	156.00	0.09		
<i>Total</i>	25.11	163.00			

Table 13 Tukey's post-hoc test for plot scale PAI_e values. Significant *I-J* mean differences are bolded. The mean difference is significant at the 0.05 level. PAI_d derived values denoted with *.

<i>PAI_e</i>					<i>95% Confidence Interval</i>	
<i>Location (I)</i>	<i>Location (J)</i>	<i>Mean Difference (I-J)</i>	<i>Std. Err.</i>	<i>Significance</i>	<i>Lower</i>	<i>Upper</i>
1	2	0.37	0.07	0.00	0.14	0.60
	3	0.22	0.11	0.47	-0.11	0.55
	4	0.02	0.09	1.00	-0.25	0.28
	5	0.09	0.12	1.00	-0.29	0.47
	6	-0.27	0.08	0.02	-0.51	-0.03
	7	-0.32	0.08	0.01	-0.58	-0.06
	8*	-0.37	0.08	0.00	-0.63	-0.11
2	1	-0.37	0.07	0.00	-0.60	-0.14
	3	-0.15	0.11	0.85	-0.49	0.18
	4	-0.36	0.09	0.00	-0.63	-0.08
	5	-0.28	0.12	0.32	-0.67	0.10
	6	-0.64	0.08	0.00	-0.89	-0.40
	7	-0.69	0.09	0.00	-0.96	-0.43
	8*	-0.74	0.09	0.00	-1.00	-0.48

3	1	-0.22	0.11	0.47	-0.55	0.11
	2	0.15	0.11	0.85	-0.18	0.49
	4	-0.20	0.12	0.68	-0.56	0.16
	5	-0.13	0.15	0.99	-0.58	0.32
	6	-0.49	0.11	0.00	-0.83	-0.15
	7	-0.54	0.12	0.00	-0.90	-0.19
	8*	-0.59	0.12	0.00	-0.94	-0.23
4	1	-0.02	0.09	1.00	-0.28	0.25
	2	0.36	0.09	0.00	0.08	0.63
	3	0.20	0.12	0.68	-0.16	0.56
	5	0.07	0.13	1.00	-0.34	0.48
	6	-0.29	0.09	0.05	-0.57	0.00
	7	-0.34	0.10	0.01	-0.64	-0.04
	8*	-0.38	0.10	0.00	-0.68	-0.09
5	1	-0.09	0.12	1.00	-0.47	0.29
	2	0.28	0.12	0.32	-0.10	0.67
	3	0.13	0.15	0.99	-0.32	0.58
	4	-0.07	0.13	1.00	-0.48	0.34
	6	-0.36	0.13	0.10	-0.75	0.03
	7	-0.41	0.13	0.04	-0.81	-0.01
	8*	-0.46	0.13	0.02	-0.86	-0.05
6	1	0.27	0.08	0.02	0.03	0.51
	2	0.64	0.08	0.00	0.40	0.89
	3	0.49	0.11	0.00	0.15	0.83
	4	0.29	0.09	0.05	0.00	0.57
	5	0.36	0.13	0.10	-0.03	0.75
	7	-0.05	0.09	1.00	-0.33	0.22
	8*	-0.10	0.09	0.96	-0.37	0.18
7	1	0.32	0.08	0.01	0.06	0.58
	2	0.69	0.09	0.00	0.43	0.96
	3	0.54	0.12	0.00	0.19	0.90
	4	0.34	0.10	0.01	0.04	0.64
	5	0.41	0.13	0.04	0.01	0.81
	6	0.05	0.09	1.00	-0.22	0.33
	8*	-0.04	0.09	1.00	-0.33	0.25
8*	1	0.37	0.08	0.00	0.11	0.63
	2	0.74	0.09	0.00	0.48	1.00
	3	0.59	0.12	0.00	0.23	0.94
	4	0.38	0.10	0.00	0.09	0.68
	5	0.46	0.13	0.02	0.05	0.86
	6	0.10	0.09	0.96	-0.18	0.37
	7	0.04	0.09	1.00	-0.25	0.33

Descriptive statistics for all ALA_e values can be found in Table 14. Table 15 presents the one-tailed (ANOVA) results for ALA_e for all field sites (latitude gradient) showing that site-specific ALA_e means were statistically significantly different from one another ($p \leq 0.05$, $F=5.48$); however, unlike PAI_e, ALA_e did not show a latitudinal gradient (i.e. pattern). Subgroup means compared using a Tukey's post-hoc analysis (Table 16) showed that ALA_e measurements for Richardson Mountains (2013 and 2014) were not significantly different from one another. However, the Banks Island ALA_e values showed the greatest significant differences when compared to all other sites.

Overall, ALA_e values for all sites ranged from 10.29° to 79.92° with a mean of 52.28°. ALA_e values were used across all sites to parametrize the leaf and canopy physical models in Chapters 6 and 7.

Table 14 Descriptive statistics for ALA_e values for all field sites for the plot level.

ALA _e		95% Confidence Interval						
Site	n	Mean	Std. Dev.	Std. Err.	Lower	Upper	Min	Max
1.Herschel Island 2011	33	51.36	8.08	1.41	48.50	54.23	24.07	63.54
2.Banks Island 2012	31	61.44	13.50	2.43	56.49	66.39	14.29	78.23
3.Richards Island 2012	10	40.53	28.05	8.87	20.46	60.59	11.30	79.92
4. Tuktoyaktuk 2012	7	41.98	21.43	8.10	22.16	61.80	10.29	69.73
5. Richards Island 2013	18	53.50	6.47	1.52	50.28	56.71	38.17	63.20
6.Richardson Mountains 2013	25	53.94	9.49	1.90	50.02	57.86	34.28	71.68
7.Richardson Mountains 2014	20	45.92	13.21	2.95	39.73	52.09	20.60	66.37
Total	144	52.28	14.30	1.19	49.93	54.64	10.29	79.92

Table 15 ANOVA results for ALA_e comparisons by field site at the plot scale.

ALA _e	Sum of squares	Degrees of freedom	Mean square	F	Significance
Between groups	5659.69	6.00	943.28	5.48	0.00
Within groups	23580.53	137.00	172.12		
Total	29240.21	143.00			

Table 16 Tukey's post-hoc test for plot scale ALA_e values. Significant *I-J* mean differences are bolded. The mean difference is significant at the 0.05 level.

ALA _e		95% Confidence Interval					
Location (I)	Location (J)	Mean Difference (I-J)	Std. Err.	Significance	Lower	Upper	
1	2	-10.08	3.28	0.04	-19.90	-0.26	
	3	10.84	4.74	0.26	-3.33	25.01	
	4	9.38	5.46	0.61	-6.96	25.72	
	5	-2.13	3.84	1.00	-13.64	9.37	
	6	-2.58	3.48	0.99	-12.99	7.83	
	7	5.45	3.72	0.76	-5.67	16.58	
2	1	10.08	3.28	0.04	0.26	19.90	
	3	20.91	4.77	0.00	6.64	35.19	
	4	19.46	5.49	0.01	3.03	35.89	
	5	7.94	3.89	0.39	-3.69	19.58	
	6	7.50	3.53	0.34	-3.06	18.05	
	7	15.53	3.76	0.00	4.27	26.79	
3	1	-10.84	4.74	0.26	-25.01	3.33	
	2	-20.91	4.77	0.00	-35.19	-6.64	
	4	-1.46	6.47	1.00	-20.80	17.89	
	5	-12.97	5.17	0.17	-28.46	2.51	
	6	-13.42	4.91	0.10	-28.11	1.27	
	7	-5.39	5.08	0.94	-20.59	9.82	
4	1	-9.38	5.46	0.61	-25.72	6.96	
	2	-19.46	5.49	0.01	-35.89	-3.03	

	3	1.46	6.47	1.00	-17.89	20.80
	5	-11.52	5.84	0.44	-29.00	5.97
	6	-11.96	5.61	0.34	-28.75	4.83
	7	-3.93	5.76	0.99	-21.17	13.31
5	1	2.13	3.84	1.00	-9.37	13.64
	2	-7.94	3.89	0.39	-19.58	3.69
	3	12.97	5.17	0.17	-2.51	28.46
	4	11.52	5.84	0.44	-5.97	29.00
	6	-0.44	4.06	1.00	-12.58	11.69
	7	7.59	4.26	0.56	-5.17	20.34
6	1	2.58	3.48	0.99	-7.83	12.99
	2	-7.50	3.53	0.34	-18.05	3.06
	3	13.42	4.91	0.10	-1.27	28.11
	4	11.96	5.61	0.34	-4.83	28.75
	5	0.44	4.06	1.00	-11.69	12.58
	7	8.03	3.94	0.39	-3.75	19.81
7	1	-5.45	3.72	0.76	-16.58	5.67
	2	-15.53	3.76	0.00	-26.79	-4.27
	3	5.39	5.08	0.94	-9.82	20.59
	4	3.93	5.76	0.99	-13.31	21.17
	5	-7.59	4.26	0.56	-20.34	5.17
	6	-8.03	3.94	0.39	-19.81	3.75

4.3.4. Comparison of effective canopy chlorophyll content (CCC_e)

The effective canopy chlorophyll content (CCC_e , g/m²) was determined by multiplying the LCC (µg/cm²) values by the corresponding PAI_e (m²/m²) values. The subplot scale (i.e. 1 m²) CCC_e descriptive statistics are shown in Table 17. Results of the ANOVA (Table 18) showed that, as expected from the PAI results, mean CCC_e was significantly different across the study areas ($p \leq 0.05$, $F=129.03$). Tukey's post-hoc analysis of subgroup means showed no significant difference ($p \geq 0.05$) between CCC_e measurements derived from PAI_d or PAI_e for the Richardson Mountains (2014) field site (Table 19). However, there were significant differences ($p \leq 0.05$) in CCC_e for the Richardson Mountains 2013 and 2014 seasons, a result that suggests that sampling time of year can play a large role in CCC_e estimates (July 18th to 22nd, 2013 leaf chlorophyll samples vs. July 25th to August 5th, 2014)

Table 17 Descriptive statistics for CCC_e values for all field sites for the plot level. PAI_d derived values denoted with *.

CCC _e (g/m ²)					95% Confidence Interval			
Site	n	Mean	Std. Dev.	Std. Err.	Lower	Upper	Min	Max
1.Herschel Island 2011	693	0.29	0.13	0.01	0.28	0.30	0.06	0.89
2.Banks Island 2012	520	0.18	0.10	0.00	0.17	0.19	0.01	0.65
3.Richards Island 2012	34	0.21	0.08	0.01	0.18	0.24	0.10	0.40
4.Tuktoyaktuk 2012	52	0.27	0.15	0.02	0.23	0.32	0.05	0.76
5.Richards Island 2013	162	0.27	0.12	0.01	0.25	0.29	0.05	0.90
6.Richardson Mountains 2013	225	0.40	0.13	0.01	0.38	0.41	0.15	0.83
7.Richardson Mountains 2014	99	0.47	0.18	0.02	0.43	0.50	0.11	0.80
8.Richardson Mountains 2014*	99	0.48	0.23	0.02	0.43	0.53	0.04	0.99
Total	1884	0.29	0.16	0.00	0.28	0.29	0.01	0.99

Table 18 ANOVA results for CCC_e subplot scale measurements. Results are significant at the 0.05 level.

CCC _e	Sum of squares	Degrees of freedom	Mean square	F	Significance
Between groups	16.07	7.00	2.30	129.03	0.00
Within groups	33.38	1876.00	0.02		
Total	49.44	1883.00			

Table 19 Tukey's post-hoc test comparing CCC_e subplot values. Significant *I-J* mean differences are bolded. The mean difference is significant at the 0.05 level. PAI_d derived values denoted with *.

CCC _e					95% Confidence Interval	
Location (I)	Location (J)	Mean Difference (I-J)	Std. Err.	Significance	Lower	Upper
1	2	0.11	0.01	0.00	0.09	0.13
	3	0.07	0.02	0.03	0.00	0.15
	4	0.01	0.02	1.00	-0.05	0.07
	5	0.01	0.01	0.91	-0.02	0.05
	6	-0.11	0.01	0.00	-0.14	-0.08
	7	-0.18	0.01	0.00	-0.22	-0.13
	8*	-0.19	0.01	0.00	-0.24	-0.15
2	1	-0.11	0.01	0.00	-0.13	-0.09
	3	-0.04	0.02	0.80	-0.11	0.04
	4	-0.10	0.02	0.00	-0.16	-0.04
	5	-0.10	0.01	0.00	-0.13	-0.06
	6	-0.22	0.01	0.00	-0.25	-0.19
	7	-0.29	0.01	0.00	-0.33	-0.24
	8*	-0.30	0.01	0.00	-0.35	-0.26
3	1	-0.07	0.02	0.03	-0.15	0.00
	2	0.04	0.02	0.80	-0.04	0.11
	4	-0.06	0.03	0.41	-0.15	0.03
	5	-0.06	0.03	0.25	-0.14	0.02
	6	-0.18	0.02	0.00	-0.26	-0.11
	7	-0.25	0.03	0.00	-0.33	-0.17
	8*	-0.27	0.03	0.00	-0.35	-0.19
4	1	-0.01	0.02	1.00	-0.07	0.05
	2	0.10	0.02	0.00	0.04	0.16
	3	0.06	0.03	0.41	-0.03	0.15
	5	0.00	0.02	1.00	-0.06	0.07
	6	-0.12	0.02	0.00	-0.18	-0.06
	7	-0.19	0.02	0.00	-0.26	-0.12
	8*	-0.21	0.02	0.00	-0.28	-0.14

5	1	-0.01	0.01	0.91	-0.05	0.02
	2	0.10	0.01	0.00	0.06	0.13
	3	0.06	0.03	0.25	-0.02	0.14
	4	0.00	0.02	1.00	-0.07	0.06
	6	-0.12	0.01	0.00	-0.16	-0.08
	7	-0.19	0.02	0.00	-0.24	-0.14
	8*	-0.21	0.02	0.00	-0.26	-0.16
6	1	0.11	0.01	0.00	0.08	0.14
	2	0.22	0.01	0.00	0.19	0.25
	3	0.18	0.02	0.00	0.11	0.26
	4	0.12	0.02	0.00	0.06	0.18
	5	0.12	0.01	0.00	0.08	0.16
	7	-0.07	0.02	0.00	-0.12	-0.02
	8*	-0.09	0.02	0.00	-0.13	-0.04
7	1	0.18	0.01	0.00	0.13	0.22
	2	0.29	0.01	0.00	0.24	0.33
	3	0.25	0.03	0.00	0.17	0.33
	4	0.19	0.02	0.00	0.12	0.26
	5	0.19	0.02	0.00	0.14	0.24
	6	0.07	0.02	0.00	0.02	0.12
	8*	-0.02	0.02	0.99	-0.07	0.04
8*	1	0.19	0.01	0.00	0.15	0.24
	2	0.30	0.01	0.00	0.26	0.35
	3	0.27	0.03	0.00	0.19	0.35
	4	0.21	0.02	0.00	0.14	0.28
	5	0.21	0.02	0.00	0.16	0.26
	6	0.09	0.02	0.00	0.04	0.13
	7	0.02	0.02	0.99	-0.04	0.07

The CCC_e values were subsequently compared at the plot level to determine if the same significant differences existed between sites when subplot variability was removed. Descriptive statistics for the plot scale CCC_e means are shown in Table 20. Results of the ANOVA (Table 21) showed that site means were statistically significantly different across the study areas ($p \leq 0.05$, $F=20.11$), where a lower F value can be seen. Tukey's post-hoc comparison of the subgroup means showed no significant difference ($p \geq 0.05$) between the CCC_e measurements for the PAI_d and PAI_e derived estimates of CCC_e for the Richardson Mountains (2014) field site (Table 22). Furthermore, there were no significant differences ($p \leq 0.05$) between the CCC_e values for the Richardson Mountains 2013 and 2014 seasons, a result that suggests that it is best to aggregate subplot (1 m²) scale data to the plot level to reduce variability when conducting larger spatial scale/extent analyses (e.g. moderate resolution remote sensing studies).

Table 20 Descriptive statistics for CCC_e for all field sites for plot scale measurements. PAI_d derived values denoted with *.

CCC _e (g/m ²)		95% Confidence Interval						
Site	n	Mean	Std. Dev.	Std. Err.	Lower	Upper	Min	Max
1.Herschel Island 2011	33	0.29	0.10	0.02	0.25	0.32	0.14	0.51
2.Banks Island 2012	31	0.15	0.10	0.02	0.11	0.18	0.00	0.38
3.Richards Island 2012	10	0.22	0.09	0.03	0.16	0.29	0.11	0.40
4.Tuktoyaktuk 2012	7	0.26	0.14	0.05	0.13	0.39	0.11	0.51
5.Richards Island 2013	18	0.27	0.10	0.02	0.22	0.32	0.09	0.58
6.Richardson Mountains 2013	25	0.40	0.11	0.02	0.35	0.44	0.21	0.63
7.Richardson Mountains 2014	20	0.47	0.18	0.04	0.38	0.55	0.13	0.77
8.Richardson Mountains 2014*	20	0.48	0.17	0.04	0.40	0.56	0.13	0.72
Total	164	0.32	0.17	0.01	0.29	0.34	0.00	0.77

Table 21 ANOVA results for CCC_e comparisons by field site at the plot scale. Results are significant at the 0.05 level.

CCC _e	Sum of squares	Degrees of freedom	Mean square	F	Significance
Between groups	2.22	7.00	0.32	20.11	0.00
Within groups	2.45	156.00	0.02		
Total	4.67	163.00			

Table 22 Tukey's post-hoc test for plot scale CCC_e measurements. Significant *I-J* mean differences are bolded. The mean difference is significant at the 0.05 level. PAI_d derived values denoted with *.

CCC _e		95% Confidence Interval				
Location (I)	Location (J)	Mean Difference (I-J)	Std. Err.	Significance	Lower	Upper
1	2	0.14	0.03	0.00	0.04	0.24
	3	0.06	0.05	0.87	-0.08	0.20
	4	0.03	0.05	1.00	-0.13	0.19
	5	0.01	0.04	1.00	-0.10	0.13
	6	-0.11	0.03	0.03	-0.21	-0.01
	7	-0.18	0.04	0.00	-0.29	-0.07
	8	-0.19	0.04	0.00	-0.30	-0.08
2	1	-0.14	0.03	0.00	-0.24	-0.04
	3	-0.08	0.05	0.67	-0.22	0.06
	4	-0.11	0.05	0.38	-0.27	0.05
	5	-0.13	0.04	0.02	-0.24	-0.01
	6	-0.25	0.03	0.00	-0.35	-0.15
	7	-0.32	0.04	0.00	-0.43	-0.21
	8	-0.33	0.04	0.00	-0.45	-0.22
3	1	-0.06	0.05	0.87	-0.20	0.08
	2	0.08	0.05	0.67	-0.06	0.22
	4	-0.04	0.06	1.00	-0.23	0.15
	5	-0.05	0.05	0.98	-0.20	0.10
	6	-0.17	0.05	0.01	-0.32	-0.03
	7	-0.24	0.05	0.00	-0.39	-0.09
	8	-0.26	0.05	0.00	-0.41	-0.11
4	1	-0.03	0.05	1.00	-0.19	0.13
	2	0.11	0.05	0.38	-0.05	0.27
	3	0.04	0.06	1.00	-0.15	0.23
	5	-0.01	0.06	1.00	-0.18	0.16
	6	-0.14	0.05	0.19	-0.30	0.03
	7	-0.21	0.06	0.01	-0.38	-0.04
	8	-0.22	0.06	0.00	-0.39	-0.05

5	1	-0.01	0.04	1.00	-0.13	0.10
	2	0.13	0.04	0.02	0.01	0.24
	3	0.05	0.05	0.98	-0.10	0.20
	4	0.01	0.06	1.00	-0.16	0.18
	6	-0.12	0.04	0.04	-0.24	0.00
	7	-0.19	0.04	0.00	-0.32	-0.07
	8	-0.21	0.04	0.00	-0.33	-0.08
6	1	0.11	0.03	0.03	0.01	0.21
	2	0.25	0.03	0.00	0.15	0.35
	3	0.17	0.05	0.01	0.03	0.32
	4	0.14	0.05	0.19	-0.03	0.30
	5	0.12	0.04	0.04	0.00	0.24
	7	-0.07	0.04	0.57	-0.19	0.04
	8	-0.09	0.04	0.32	-0.20	0.03
7	1	0.18	0.04	0.00	0.07	0.29
	2	0.32	0.04	0.00	0.21	0.43
	3	0.24	0.05	0.00	0.09	0.39
	4	0.21	0.06	0.01	0.04	0.38
	5	0.19	0.04	0.00	0.07	0.32
	6	0.07	0.04	0.57	-0.04	0.19
	8	-0.01	0.04	1.00	-0.14	0.11
8*	1	0.19	0.04	0.00	0.08	0.30
	2	0.33	0.04	0.00	0.22	0.45
	3	0.26	0.05	0.00	0.11	0.41
	4	0.22	0.06	0.00	0.05	0.39
	5	0.21	0.04	0.00	0.08	0.33
	6	0.09	0.04	0.32	-0.03	0.20
	7	0.01	0.04	1.00	-0.11	0.14

The PAI_e derived CCC_e values are visualized in Figure 34. There is a noticeable downward trend in CCC_e values when progressing northward, which is likely attributable to sparser canopies (lower gap fraction and PAI_e) rather than to diminishing LCC values, as high LCC values at northerly sites were observed in some data. Mean CCC_e values ranged from ~0.18 g/m² at high latitudes, through 0.26 g/m² at mid-latitudes, to 0.45 g/m² at the lowest latitudes.

Figure 34 Subplot-scale CCC_e (g/m²) plotted for each of the field sites per latitude.

4.4. Discussion and Conclusion

The hemispherical photography results showed that it is possible to model and measure PAI_c and PAI_t in tundra environments. In addition, CAN-EYE used in combination with DHP can provide relevant and much needed information on canopy structure (e.g. ALA, *f*Cover, gap fraction, and clumping index). Measurements with DHP are quick and easy and capable of being completed over larger spatial domains in relatively short time-periods, thus making the technique valuable for remote fieldwork. The CAN-EYE methodology provides a relatively efficient workflow as compared to the destructive approaches used in this study, given that up to 25 photographs can be processed at one time. However, as Demarez et al. (2008) have indicated, to obtain the best possible measurements of gap fraction and associated estimates of PAI, several considerations need to be made. (1) Gap fractions need to be representative of the entire canopy; this is particularly true for Arctic canopies since they are extremely spatially heterogeneous at the

1 m² scale. (2) The optimal distance between the camera and canopy should be greater than 1 m; in this study 1.5 m was used and found to be suitable for accurate characterization of canopy parameters/variables. (3) When feasible, photographs of the canopy should be made under overcast conditions to minimize shadows since they may lead to uncertainties and over estimates of gap fractions. This was found to be especially important in hummocky terrain where shadow contamination can be prevalent under sunny conditions and shadow occurrence augmented due to the generally low sun angle at northern latitudes. However, it is possible to post-process images to remove some shadow, particularly if DHP images are acquired in raw format, fixed for exposure issues and then converted to the highest quality JPEG before processing with CAN-EYE. This study did not evaluate systematic error caused by or due to changing environmental conditions; the strong relationships of DHP-derived PAI with the reference PAI_d measurements were deemed to be sufficient to warrant the use of PAI_e estimates for all field sites in subsequent physical modelling (Chapters 5-7). It is recommended that further studies using DHP and CAN-EYE in Arctic tundra investigate canopy to sensor distance, sky conditions (sun/sensor geometry), VZA restrictions (e.g. what is the optimal COI for use in tundra?), and investigate optimal time of year as PAI is expected to change throughout the growing season. Additional methods to measure PAI, such as extraction at 57.5° (retrieval of PAI_e is independent of ALA), were not investigated but have shown promise in other studies (Demarez et al., 2008).

In this study, two methods of PAI estimation were compared against destructive measurements of PAI. It was demonstrated that the use of the clumping index (PAI_t) was not as good at predicting PAI_d as using effective PAI (PAI_e) calculated within a 45° COI. Analysis of derived PAI_e values for these Arctic sites revealed overall low values (0.00 to 2.50) that generally decrease with increasing latitude, as biomass per unit area diminishes. Similarly, canopy gap fraction was shown

to increase with latitude as canopy biomass structural complexity and spatial coverage decrease. Combining measured leaf chlorophyll (Chapter 3) with PAI_e showed that, as for PAI_e , the resulting canopy level chlorophyll (CCC_e) values also decreased with increasing latitude.

Destructive vegetation sampling followed by PAI measurement in the laboratory was shown to be a simple and straight forward approach that only required a pair of shears, camera, white background cloth, and software/computer to threshold the resulting images. However, in the Arctic with large travel distances to remote locations, this approach is not feasible for data acquisition over many sites. Therefore, it was used as a means to evaluate DHP-derived PAI at a single site, leading to the conclusion that DHP-derived PAI_e was a suitable metric for measurement at all sites of this study. PAI_d values for the Richardson Mountains site subplot level ranged from 0.12 to 2.63 and from 0.35 to 1.74 when averaged at the plot scale. Like the process employed by CAN-EYE, reliable measurements of destructive PAI are only attainable when subplot measurements are averaged across larger spatial extents to account for the high degree of spatial variability at the subplot ($1m^2$) scale. While PAI_d was used as the reference data, it is not an absolute reference in itself. Error sources include: (1) vegetation may not be spread out evenly when photographing (i.e. ensuring no overlap), which could lead to under-estimation, and (2) vegetation and background material (e.g. shadows) could be misclassified leading to either over- or under-estimation.

Finally, the distinct latitudinal gradient in vegetation cover and PAI over the study sites of this research was beneficial as it allowed for analysis over a range of representative Arctic ecosystem conditions. However, sampling within a given study site should also be conducted over a gradient of low to high canopy densities in order to provide a representative range of the existing environmental conditions. If sampling is conducted entirely within a homogeneous area, it is expected that the results will not provide suitable predictive power outside of that area.

Chapter 5. Evaluation of Empirical Parametric and Non-Parametric Biochemical and Biophysical Retrieval Methods: Field Scale Analysis across an Arctic Bioclimatic Gradient

Abstract

Estimating the spatial distribution of foliar biochemicals with optical instrumentation (i.e. remote sensing) can serve as an important approach for monitoring plant community characteristics, as such measurements can provide insight into ecosystem composition, disturbance, and/or stress caused by changing environmental conditions. Warming in the Arctic has resulted in changes to the distribution and composition of Arctic vegetation communities, and many of these changes may not be detectable by broadband sensors. Vegetation monitoring in Arctic regions has been mostly accomplished through classification and empirical parametric biophysical variable estimation using nadir looking broadband instruments at coarse spatial scales. Recent and future remote sensing developments include multi-angle, high spatial resolution spectroscopic imagers capable of characterizing angular reflectance across the spectrum in many contiguous narrow bands. Multi-angle optical instruments such as CHRIS/PROBA help to exploit additional reflectance information over nadir looking instruments, thus potentially providing greater insight and understanding into the independent variables contributing to reflectance anisotropy. In this study, the retrieval of leaf and canopy biochemical (i.e. leaf chlorophyll content, LCC, $\mu\text{g}/\text{cm}^2$; canopy chlorophyll content [$\text{CCC}_e = \text{LCC} \times \text{PAI}_e$], g/m^2) and biophysical (i.e. effective plant area index, PAI_e , m^2/m^2) variables from multi-angle, ground-based spectroradiometry was conducted. Field reflectance data were acquired with an ASD FieldSpec Handheld (305 nm to 1075 nm) and used to simulate CHRIS/PROBA (411-997 nm) satellite spectra at two spatial resolutions (1 m x 1 m and 90 m x 90 m). Multi-angle spectral measurements

were taken in the field that corresponded to the descending pathway ($\sim 97.84^\circ$ inclination) and view zenith angles (VZA) (-55° , -36° , 0° , $+36^\circ$, $+55^\circ$) of CHRIS/PROBA. Various vegetation indices (VIs) were evaluated, including those that are broadly defined such as the simple ratio (e.g., $SR = NIR/R$), for which optimal narrowband combinations were determined using iterative analysis, and pre-defined narrowband VIs, which were tested using their published bands. The overall goal of this study was to develop an understanding of the potential of VIs and empirical retrieval methods at the field scale. This is combined with a similar study using reflectance-based physical modelling (Chapter 6) to develop an appropriate approach for subsequent satellite-based retrieval of these biochemical-biophysical variables (Chapter 7). Biochemical-biophysical variable measurements were made between 2011 and 2014 across a bioclimatic gradient in the Western Canadian Arctic. Relationships of existing narrowband VIs with the biophysical-chemical variables were evaluated using parametric linear regression; this analysis was conducted across all VZAs, spectral datasets (subsets), and spatial configurations at each of the field sites. Similarly, the non-parametric non-linear machine learning regression algorithm Gaussian Processes Regression (GPR) was implemented using full spectrum data to investigate its ability to predict LCC, PAI_e , and CCC_e for the same datasets. The linear regression results indicate that the simple ratio ($SR = NIR/R$) was the most useful VI for retrieving LCC, PAI_e , and CCC_e over all sites and data configurations (mean $r^2_{cv}=0.51$, $NRMSE_{cv}=0.15$; cv = cross validated; $NRMSE$ = normalized RMSE) with optimal bands falling between 642 and 762 nm, whereas the revised optimized soil adjusted vegetation index (ROSAVI) with predefined bands of 705 and 750 nm was the best performing narrowband VI (mean $r^2_{cv}=0.45$, $NRMSE_{cv}=0.18$). The GPR approach produced similar results for predicting LCC, PAI_e , and CCC_e over all sites and data configurations (mean $r^2_{cv}=0.52$, $NRMSE_{cv}=0.17$), with optimal bands being between 608 to 736 nm. Best overall

modelling results based on r^2_{cv} were achieved with the GPR approach at the plot scale (mean $r^2_{cv}=0.62$, across all VZAs), followed by the SR VI (mean $r^2_{cv}=0.58$, across all VZAs) and finally the ROSAVI (mean $r^2_{cv}=0.54$, across all VZAs); however, best predictive performance was achieved by SR (mean $NRMSE_{cv}=0.12$) followed by, GPR (mean $NRMSE_{cv}=0.16$) and ROSAVI (mean $NRMSE_{cv}=0.16$). All retrieval methods showed optimal band performance related to pigment absorption regions in the visible and structural reflectance effects in the NIR (along the red-edge slope); however, all variables showed some degree of spectral covariation resulting in the selection of spectral bands outside of known absorption ranges. The overall best performing VZA for both parametric and non-parametric retrieval methods was -55° (mean $r^2_{cv}=0.52$); however, results were not sufficiently different than for the other VZAs to recommend monitoring of these vegetation variables at off-nadir angles.

5.1. Introduction

Quantitative empirically-based retrieval methods used for the estimation of vegetation biogeophysical characteristics from optical remote sensing data are the basis for a variety of ecological applications (Darvishzadeh et al., 2008a; Ustin et al., 2009; Verrelst et al., 2015a,b; Verrelst et al., 2016). Optical earth observing satellites equipped with high spatial and increasingly high spectral resolution sensors (e.g. imaging spectrometers) are enabling enhanced empirical retrieval capabilities for monitoring plant variables, such as pigment biochemistry (e.g. leaf chlorophyll content, LCC; and canopy chlorophyll content, CCC), non-pigment biochemistry (nitrogen, lignin, and cellulose) and canopy biophysical attributes (e.g. canopy gap fraction, plant area index, PAI) (Darvishzadeh et al., 2008a; Blackburn et al., 2007; Dorigo et al., 2007; Ustin et al., 2009; Kokaly et al., 2009; Verrelst et al., 2015a,b; Verrelst et al., 2016).

With increases to data availability and spectral data dimensionality, the methodological challenges also increase. Thus, large remote sensing data volumes require enhanced and robust retrieval techniques. Unfortunately, imaging spectroscopy data often contain highly correlated and noisy spectral bands that create statistical problems (Verrelst et al., 2015a,b). When empirical models are fitted with multi-collinear spectral data they are susceptible to overfitting, and consequently, prediction/retrieval accuracy and model transferability can suffer (Curran, 1989; Grossman et al., 1996; Verrelst et al., 2016). Spectral dimensionality can be reduced to determine optimal narrow spectral bands (an advantage over broadband multispectral imaging), either through feature reduction techniques (e.g. Arenas-Garcia et al., 2013; Verrelst et al., 2016), or through carefully chosen spectral regions that best describe the absorption and reflectance properties of the variable of interest (e.g. based on expert knowledge). Regardless of method, the selection of the best spectral predictor variable from a large feature-rich dataset is considered a necessary step for the selection of the optimal predictive model. With respect to purely empirical retrieval methodologies, two statistical approaches are commonly employed to find the optimal predictor features from spectroscopic data: parametric and non-parametric regression methods. The focus here is on parametric linear regression based on vegetation indices (VIs) (as described in Section 2.2.2.1.) and non-parametric non-linear machine learning regression algorithms (MLRAs) (as described in Section 2.2.2.2.).

Although not as commonly used as linear parametric models, the variety and availability of non-linear non-parametric MLRAs has increased in recent years (Verrelst et al., 2015b; Verrelst et al., 2016). The methodological advantage of non-linear, non-parametric MLRA methods over linear-parametric methods is their capability of capturing and handling the non-linear relationships between predictor and dependent variables without knowing their underlying data distributions

(Verrelst et al., 2015b; Verrelst et al., 2016). Given this, MLRAs have been shown to work well with a variety of data types such as hyper-dimensional feature-rich spectral data that exhibit a high degree of multicollinearity (e.g. Verrelst et al., 2015a,b). Studies using MLRAs have demonstrated that Gaussian processes regression (GPR) (Rasmussen & Williams, 2006) is capable of outperforming other MLRAs for the retrieval of vegetation biochemical and biophysical variables from airborne and satellite imaging spectroscopy data (Rivera et al., 2014a, Verrelst et al., 2012b, Verrelst et al., 2015; Verrelst et al., 2016; Camps-Valls et al., 2016). To fully test the usefulness of GPR, it is imperative to test it across various environments and with various sensor data types (Verrelst et al., 2016). It is also imperative to test such methods against common/traditional methods (e.g. linear regression using VIs) with replicate datasets. Furthermore, a comparison of these methods for quantitative retrievals of vegetation biophysical and biochemical quantities has not been fully explored across naturally occurring ecosystems including Arctic tundra ecosystems.

A review of the Arctic remote sensing literature shows that all spectroscopic studies have been conducted at the field scale (Liu et al., 2017; Bratsch et al., 2016; Buchhorn et al., 2013; Davidson et al., 2016; Hope et al., 1993; Huemmrich et al., 2013; Kushida et al., 2009, 2015; Laidler et al., 2008; Riedel et al., 2005a,b; Ulrich et al., 2009). Classification-based studies from those listed above suggest that imaging spectroscopy sensors may provide additional capabilities over broadband instruments for vegetation mapping (Bratsch et al., 2016; Davidson et al., 2016); conclusions of these studies are typically recommendations for a set of meaningful narrow spectral bands used to map the variable in question. For example, a study conducted by Bratsch et al. (2016) used partial least squares linear regression to identify optimal spectroscopic bands for classifying four Alaskan vegetation types; important spectral features were identified in several wavelength regions such as pigment absorption in the blue and red bands and structurally related reflectance

characteristics in the red-edge (RE) and near-infrared (NIR) regions. High accuracy was achieved, and the results further emphasized that full spectrum methods show promise with highly dimensional, feature-rich spectral datasets.

Studies concerning the retrieval of biophysical and biochemical variables generally focus on correlating VIs with field measured biophysical and biochemical variables. For example, VIs such as NDVI (normalized difference vegetation index), EVI (enhanced vegetation index), and SAVI (soil adjusted vegetation index) have been used to estimate percent vegetation cover (Kushida et al., 2009; Laidler et al., 2008), biomass quantities (Kushida et al., 2009; Kushida et al., 2015; Riedel et al., 2005a,b), and leaf area index (LAI) (Riedel et al., 2005a,b; Williams 2005; Williams et al., 2008). In a recent study by Liu et al. (2017) percent vegetation cover was estimated using broadband and narrowband VIs (e.g. NDVI) with simulated Worldview 3 and Hyperion data; narrowband VIs had stronger relationships with green percent vegetation cover. Buchhorn et al. (2013) assessed the performance of the NDVI involving all possible two-band combinations within the 420 to 1100 nm range for estimating shrub biomass; results of the study showed that narrowband NDVI performed with more accuracy than broadband NDVI. Fewer biochemical studies have been conducted in the Arctic. Huemmrich et al. (2013) correlated light use efficiency (LUE) calculated from functional type cover fractions with a 3-band spectroscopic VI used as a proxy for chlorophyll concentration. The results suggested that spectroscopic remote sensing can distinguish functionally distinct vegetation types and can be used to develop regional estimates of photosynthetic LUE in tundra landscapes. Currently, there are no studies that have measured foliar biochemical quantities in the field (e.g. chlorophyll) for remote sensing retrieval purposes, and furthermore there has not been a robust comparison of spectroscopic-based retrieval methods. In

addition, there has not been a comprehensive assessment of VIs for retrieval of biochemical and biophysical variables in tundra environments.

Determining the optical properties of Arctic biomass is complicated by numerous factors, such as: (1) the assemblage of various plant types and non-vascular plants/organisms (e.g. lichen, moss, and cyanobacteria), (2) non-photosynthetic components of vegetation (e.g. woody materials, leaf litter, and senescent vegetation), (3) leaf and canopy architecture, and their spatial organization, (4) soil and substrate reflectance (e.g. organic and moisture content), and (5) illumination conditions and sensor viewing geometry (e.g. view zenith angles) (Asner, 1998; Curran, 1989; Stow et al., 2004; Feret et al., 2008; Juszak et al., 2014; Juszak et al., 2017; Liu et al., 2017). This last point is of interest since there are no studies examining the estimation/extraction of Arctic biophysical and biochemical variables, let alone studies that compare parametric to non-parametric extraction methods, using multi-angle spectroscopic data. The multi-angle approach is realized through multi-angle optical instruments such as CHRIS/PROBA (Barnsley et al., 2004). Multi-angle instruments provide the possibility to test the directional capability of variable retrieval methods (Stagakis et al., 2010; He et al., 2016; Stagakis et al., 2014; Stagakis et al., 2016; Sykioti et al., 2011; Schaepman, 2007). For example, VIs are expected to be influenced by sun-target-sensor geometry because of the wavelength dependent levels of anisotropy for various vegetation types, canopy structures, non-photosynthetic materials, background and soil reflectance, and shadowing (Kimes et al., 1985; Qi et al., 1995; Chen et al., 2003; Stagakis et al., 2010; Sykioti et al., 2011). The absence of directional testing limits the potential use of various extraction methods in Arctic environments where sun and sensor angles are often at extremes; it was therefore of great interest to explore this potential since sampling of tundra reflectance anisotropy could lead to

enhanced retrievals of biophysical and biochemical variables as in similar retrieval-based studies (Stagakis et al., 2010; Sykieti et al., 2011).

Considering the above, the primary objective of this study was to investigate multi-angle field spectroscopic data for estimating the biochemical (i.e. LCC, CCC_e) and biophysical (i.e. PAI_e) properties of Arctic vegetation across a latitudinal gradient in the Western Canadian Arctic. The secondary objective was to compare the effectiveness of parametric regression using VIs and non-parametric non-linear multivariate (i.e. GPR) retrieval methods across all VZAs and across varied field sites (i.e. the latitudinal gradient) for estimating field measured biochemical and biophysical tundra parameters/variables and for identifying optimal predictor variables (spectral bands). A sub-goal of the secondary objective was to determine the best performing VIs that could be used reliably across various data-environment scenarios. The final objective of the study was to test the effect of varying the spatial and spectral sampling scales on the prediction of field-based measurements (i.e. down-sampling the spectral data and averaging field and spectral measurements to account for larger spatial scales – variability) to understand the optimal spectral and spatial scales for multi-angle retrievals of biochemical and biophysical variables. This objective has implications for vegetation variable retrieval using CHRIS/PROBA satellite data in Chapter 7. Spectral resampling was completed in accordance with the CHRIS/PROBA sensor specifications.

5.2. Materials and Methods

5.2.1. Study areas

The study areas used for the field scale empirical analysis were based on the field locations detailed earlier in the thesis (Chapter 2). These sites included Herschel Island, YT, Banks Island, NT, Richards Island, NT, and the Richardson Mountains, YT/NT. Due to the lack of adequate

spectral measurements completed at the plot scale, the Tuktoyaktuk, NT (2012) and Richards Island, NT (2012) field sites were discarded from the analysis. All field sites were visited between July 10th and August 4th in given years between 2011 and 2014 during what is considered the peak of the growing seasons to minimize any phenological variability introduced by the short tundra growing season. Table 23 shows the date and time range that each location was sampled.

5.2.2. Ground data and spectral measurements and processing

Measurements of leaf chlorophyll content (LCC, $\mu\text{g}/\text{cm}^2$), effective plant area index (PAI_e , m^2/m^2), and effective canopy chlorophyll content (CCC_e g/m^2) were sampled at all field sites using a stratified-systematic-random sampling method as shown in Figure 35 (LCC and CCC_e) and Figure 23 (PAI_e). An in-depth description of the chlorophyll sampling and processing can be found in Chapter 3 and the description of the measurement and modelling of PAI_e can be found in Chapter 4. Within each of the subplots there existed different species compositions and relative abundances. Species varied in terms of leaf shape, leaf size, and the amount of leaves (i.e. PAI_e) and the distribution of their typical angles. Chlorophyll measurements represent the average conditions within each of the subplots (fully senescent vegetation was not sampled). All biochemical and biophysical variables hereafter assume the measurement systems above.

The central location of each 30-meter square, as seen Figure 35, was recorded using a Trimble Juno handheld GPS unit (~ 3 -meter accuracy), thus 9 GPS measurements were taken per ground plot. Plot orientation was set up to match the descending orbital path of the CHRIS/PROBA satellite ($\sim 97.84^\circ$ inclination or $\sim 7.84^\circ$ from true north) (Barnsley et al., 2004). This was accomplished using a handheld compass corrected with the Natural Resources Canada magnetic declination calculator prior to field work. Plot orientation was then checked against GPS position and refined accordingly.

Figure 35 LCC, PAI_c, and spectral sampling strategy for all study areas.

In total 4 spectral datasets were used for analysis: ASD-subplot reflectance measured at the 1 m² subplot scale and averaged to the plot scale; simulated CHRIS/PROBA spectra at the 1 m² subplot scale and at the plot scale. The simulated spectral subset was based upon the Mode-1 spectral characteristics of the CHRIS/PROBA satellite: 62 spectral bands measuring the visible spectrum from 400 nm to 1050 nm with spectral sampling of approximately ~10 nm. All spectral measurements were acquired with an ASD FieldSpec handheld spectroradiometer (Analytical Spectral Devices, Inc. Boulder, USA). The FieldSpec is a highly portable, general purpose

spectroradiometer useful for many applications requiring either the relative or absolute measurement of light energy. The instrument measures the VNIR (visible near-infrared) spectrum within a range from 305 to 1075 nm with a 512-channel silicon photodiode array overlaid with an order separation filter (ASD, 2008). Each channel is geometrically positioned to receive light within a narrow 1.6 nm nominal bandwidth. It has a spectral resolution of approximately 3 nm at around 700 nm. For each spectral measurement taken in the field, signal noise from the spectrometer was reduced through spectrum averaging; the spectrometer capture software RS3 (Analytical Spectral Devices, Inc. Boulder, USA) was set up to automatically average 10 repeated measurements. Within the literature it has been shown that a sample average of around 10 to 25 is sufficient for most materials (ASD, 2008). Absolute reference spectra were taken over a portable Spectralon panel (Labsphere Inc., North Sutton, New Hampshire, USA) before measurements in each plot/subplot to account for changing atmospheric conditions. Spectralon is a fluoropolymer which has the highest known diffuse reflectance over the visible-NIR spectrum (Georgiev & Butler, 2007). Ground-based radiance measurements are divided by the white panel radiance measurements within the software to derive spectral reflectance.

Spectral measurements were taken using the same stratified-systematic sampling approach as shown in Figure 35. A total of 2667 1 m² subplots were measured across the bioclimatic gradient across all five field sites. Some measurements were averaged in the field, thus resulting in a total of 1699 subplots. Within each of the 1 m² subplots, five spectral measurements (each comprised of 10 spectra that had been averaged) were taken at a height of 1.5 m using a 10° fore optic with a ground field of view (GFOV) of ~26 cm at 1.5 m height (at nadir). The placement of the GFOV measurements in each subplot were in accordance with Figure 36. Multiple measurement locations were used to account for spectral-spatial variability at the subplot scale. The five reflectance

measurements for each subplot were later averaged to produce one measurement; this produced a total of 21 nadir spectra per plot corresponding to the 21 white squares (small squares) in Figure 35. The GFOV of the 10° foreoptic was calculated based on the diagram in Figure 36. Equation 16 was used to determine the GFOV from nadir (i.e. perpendicular to the target).

$$y = 2(h \times \tan \alpha) \quad (16)$$

where y is the diameter of the GFOV, h is the height of the spectrometer, and α is half the foreoptic field of view (FOV). As the sensor is tilted the GFOV is increased in size when the same distance is maintained from the target (the GFOV becomes ellipsoidal). To keep a consistent measurement GFOV as possible, the height of the spectrometer was varied with off-nadir measurements (in an arc, similar in procedure to a goniometer). The diameter of the maximum GFOV calculated for the largest VZAs ($\pm 55^\circ$) (using Equation 17) was approximately ~50 cm at a height of 1 m. Although larger when off-nadir, all GFOVs were well within the boundaries of the subplots.

Figure 36 Ground field of view (GFOV) representation for ASD spectrometer measurements taken at nadir using a 10° fore optic.

Multi-angular spectral measurements were taken to correspond with the theoretical/operational view angle geometry of the CHRIS/PROBA sensor: -55° , -36° , 0° , $+36^\circ$, $+55^\circ$, where positive view angles correspond to forward scatter and negative angles to backscatter. Furthermore, angular measurements were made in accordance with the descending pathway angle of the CHRIS/PROBA sensor ($\sim 7.84^\circ$ from true north) to best simulate the expected VZA geometry. Timing of field spectral data acquisition was planned to align with CHRIS acquisitions, but this was not always possible due to weather and variable CHRIS acquisition timing. Therefore, the relative sun-sensor zenith/azimuth angles did not always match those for the CHRIS sensor.

Measurements were taken with the ASD mounted on tripod with a geared photography head that is capable of fine adjustment (Manfrotto 405 Geared Head, Cassola, Italy). Fine scale measurements of geometry were checked with a digital inclinometer with an accuracy of $\pm 0.2^\circ$ (Beall Tool Company, Newark, Ohio, USA) mounted directly to the spectroradiometer. Figure 37 shows the sensor view angle geometry measured at each subplot. It should be noted that the elliptical GFOV at off-nadir angles was not shown to maintain graphical clarity. The five angular spectra were measured and averaged per subplot, giving a total of 105 (5 x 21 locations) spectra per plot. Over the course of the four field seasons a total of $\sim 13,335$ multi-angle spectral measurements were taken across the field sites.

The sun zenith and azimuth angles for each sampling period for each site can be found in Table 23. Although a thorough analysis was not completed for the exact position/geometry of the sun in relation to the sensor, sampling each site was completed at comparable seasons and daily times to reduce inter-site sun-induced variability. The associated polar plots of the sun/sensor positions can be seen in Figure 38 below (sampling periods are shown in green; 24-hour sun positions are shown

in red). For reference, the overpass time of the CHRIS/PROBA sensor for all study sites was approximately 17:00h (± 1 hour) for the years 2011 to 2014 in the month of July.

Figure 37 Conceptual multi-angular spectral sampling technique modelled after the descending path of the CHRIS/PROBA satellite over the targets. Spectral measurements were collected at five angles (+55°, +36°, 0°, -36°, and -55°) at a descending orbital pathway of $\sim 7.84^\circ$ (relative to north). Elliptical off-nadir GFOV not shown for graphical clarity.

Table 23 Field campaign locations with associated spectra acquisition time/date, sun zenith range, and sun azimuth range.

<i>Field Site:</i>	<i>Acquisition Date</i>	<i>Acquisition Time</i>	<i>Sun Zenith Range</i>	<i>Sun Azimuth Range</i>
<i>Field campaign dates</i>	<i>Range – Field work</i>	<i>Range – Field work</i>		
Herschel Island (2011)	July 18 to July 29	11:00h to 17:00h	49.11° – 63.63°	154.72° – 257.97°
Banks Island (2012)	July 10 to July 20	10:00h to 17:00h	52.86° – 60.98°	126.71° – 244.33°
Richards Island (2013)	July 25 to August 4	10:00h to 16:00h	51.74° – 62.82°	143.38° – 246.70°
Richardson Mountains (2013)	July 18 to July 22	10:00h to 17:00h	46.59° – 64.30°	139.21° – 261.85°
Richardson Mountains (2014)	July 20 to August 5	10:00h to 17:00h	47.56° – 65.18°	139.51° – 261.38°

Figure 38 Approximate sun/sensor geometry for the four field sites. Sun position is shown using 1-hour increments for the period when measurements were taken in the field. Spectral sampling periods are shown in green and are the average times for each day. All ASD acquisition angles were taken to match those of the CHRIS/PROBA sensor with a descending orbital pathway of ~ 7.84 degrees.

All measured field spectra were filtered with the Savitzky-Golay (Savitzky & Golay, 1964) technique using a second order polynomial and 15 data points (i.e. wavelengths). This technique is widely-used in spectroscopy (Ruffin & King, 1999); it performs noise reduction while preserving the higher order moments of the original spectrum, resulting in reduced overall

distortion in the reflectance signal. It has also been shown to exhibit less distortion than moving average filtering techniques when using the same order (Ruffin & King, 1999). The coefficients used in the filtering process are the same regardless of data type; Savitzky and Golay (1964) published several tables in their original publication that can be applied directly to the smoothing and differentiations of spectra. Overly noisy portions of the spectra at both ends of the spectral range were discarded resulting in spectra between 327 and 1067 nm.

CHRIS/PROBA spectra were simulated by convolving the field spectra with estimated spectral response functions (SRFs) corresponding to the CHRIS/PROBA sensor using Equation 17 (Liang, 2005; Liu et al., 2017):

$$R(\lambda_0) = \frac{\sum_{\lambda=\lambda_1}^{\lambda=\lambda_2} R(\lambda)f(\lambda, \lambda_0)}{\sum_{\lambda=\lambda_1}^{\lambda=\lambda_2} f(\lambda, \lambda_0)} \quad (17)$$

where $R(\lambda_0)$ is the simulated spectral reflectance at a central wavelength λ_0 ; $R(\lambda)$ is the measured field spectral reflectance at wavelength λ ; $f(\lambda, \lambda_0)$ is the SRF at wavelength λ with a central wavelength λ_0 ; and $\lambda_1 - \lambda_2$ is the convolution range. Since the SRFs weren't available for the CHRIS/PROBA sensor, the SRF for each band was estimated using a Gaussian function (Liu et al., 2009; Liu et al., 2017):

$$f(\lambda, \lambda_i) = \exp\left(-\frac{(\lambda_i - \lambda)^2}{\sigma_i^2}\right) \quad (18)$$

$$\sigma_i = \frac{FWHM_i}{2\sqrt{2 \ln 2}}, i = 1, \dots, 62 \quad (19)$$

where $f(\lambda, \lambda_i)$ is the SRF at wavelength λ with a central wavelength λ_i ; and $FWHM_i$ is the full width at half maximum of band i (Equations 18 and 19). The central wavelengths and FWHM/bandwidth data for the CHRIS/PROBA sensor were obtained from Cutter (2008). Spectral

resampling was performed in the ENVI software package. Finally, spatial resampling was completed for all spectral datasets by averaging subplot spectra ($n=21$) measured across each of the 90 m x 90 m ground plots into one spectral measurement representative of that plot, providing a value representative of just less than 3 x 3 CHRIS pixels (pixel size ~34 m x 34 m at nadir). All view angles were treated as separate datasets in the parametric and non-parametric analyses.

5.2.3. Data analysis and modelling

5.2.3.1. Parametric linear regression: vegetation indices

A variety of published vegetation indices (Table 24) were computed from the five spectral datasets and compared using linear regression to the field measurements (LCC, PAI_e, and CCC_e). The VI analyses were categorized into two subsections: (1) multi-band VIs based on common spectral formulations, such as the simple ratio (SR) (Birth & McVey, 1968), and (2) predefined narrowband VIs based on previously published spectral relationships. An attempt was made to analyze the performance of a comprehensive list of VIs found throughout the remote sensing literature. Although VI analyses have been completed in the Arctic (e.g. Liu et al., 2017; Buchhorn et al., 2013; Bratsch et al., 2016), there remains a significant number of untested VIs, such as those used in grasslands and or croplands, that have not been tested for use in Arctic environments. For the analysis of the simulated CHRIS/PROBA datasets, all predefined VIs were adjusted to match the closest central wavelengths of the CHRIS/PROBA bands.

For the multi-band VIs (i.e. broadband greenness), all possible two-band combinations were explored for each VI formulation. For example, the simple ratio (SR) index is defined as (Equation 20):

$$SR = \frac{R_{\lambda_i}}{R_{\lambda_j}} \quad (20)$$

where R_{λ_i} and R_{λ_j} are the spectral reflectance values of bands i and j ; λ_i and λ_j are the wavelengths of bands i and j . Each band combination was computed for the given VI and subsequently regressed against the field variable of interest. Preliminary computation tests using three and four band VIs proved to be too time consuming so were not considered. A selection of 11 of the most common VI formulations was used (Table 24). In addition to the multi-band greenness indices, predefined narrowband indices used in a multitude of other studies were also examined (Table 24). Many of these use a similar formulation to those utilized in the multi-band analysis (e.g. SR), except they employ pre-established wavelengths previously investigated under different circumstances. The predetermined VIs are grouped by their sensitivity to greenness (chlorophyll, leaf area index), pigments (carotenoids and anthocyanins), and leaf/canopy stress and water content. A total of 84 predefined VIs were evaluated.

Selection of the optimal multi-band and predefined VI (one for each category) was based upon mean model strength (r^2) of the VI vs. LCC, PAI_e, and CCC_e relationships across all view zenith angles (VZAs), spatial scales, spectral subsets, and locations. The r^2 value was used for initial VI model assessment (multi-band and pre-defined VIs) as the vegetation variables (e.g. LCC, PAI_e, and CCC_e) possessed very different numerical ranges, as they measured different aspects of the canopy, and so RMSE (root mean square error) was not used as in other retrieval studies (Verrelst et al., 2015a). Selection of the optimal bands within the multi-band VI was conducted by calculating the weighted mean centre of the spectral space using the r^2 as the weighting. For the two-selected optimal VIs, detailed analysis of r^2 and predictive performance (RMSE) across all these data configurations is presented in the Results. RMSE was calculated using Equation 21:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (x_i - \hat{x}_i)^2} \quad (21)$$

The Normalized RMSE or NRMSE (RMSE/range of measured data) (Darvishzadeh et al., 2008a) was used to compare the overall model predictions for the individual and combined variables (i.e. LCC, PAI_c, CCC_c) at the various VZAs for the selected VIs. An NRMSE of 0.10 (10%) is commonly regarded as an accuracy threshold in an operational context (Drusch et al., 2012); however, all NRMSE values were considered. The two best performing VIs were applied in further analysis at the remote sensing scale (Chapter 7).

Table 24 Vegetation indices, proposed in the relevant literature, that were tested in the present study. Indices are sorted with respect to their original design and expected function. R_x stands for reflectance at wavelength x .

<i>Acronym</i>	<i>Index Name</i>	<i>Formulation</i>	<i>Reference</i>
<i>Broadband Greenness (*tested for each band combination, classed as multi-band)</i>			
SR	Simple Ratio	R_{nir}/R_{red}	Birth & McVey (1968)
DVI	Difference Vegetation Index	$R_{nir} - R_{red}$	Tucker (1979)
IPVI	Infrared Percentage Vegetation Index	$R_{nir}/(R_{nir} + R_{red})$	Crippen (1990)
MNLI	Modified Nonlinear Index	$((R_{nir}^2 - R_{red}) \times (1 + 0.5)) / (R_{nir}^2 + R_{red} + 0.5)$	Yang et al. (2008)
MSR	Modified Simple Ratio	$(R_{nir}/R_{red} - 1) / (\sqrt{R_{nir}/R_{red}} + 1)$	Chen (1996a)
NLI	Nonlinear Index	$(R_{nir}^2 - R_{red}) / (R_{nir}^2 + R_{red})$	Goel & Qin (1994)
SR*NDVI	Simple Ratio x NDVI	$(R_{nir}^2 - R_{red}) / (R_{nir} + R_{red}^2)$	Gong et al. (2003)
RDVI	Renormalized Difference Vegetation Index	$(R_{nir} - R_{red}) / \sqrt{R_{nir} + R_{red}}$	Roujean & Breon (1995)
SAVI	Soil Adjusted Vegetation Index	$1.5(R_{nir} - R_{red}) / (R_{nir} + R_{red} + 0.5)$	Huete (1988)
TDVI	Transformed Difference Vegetation Index	$\sqrt{0.5 + (R_{nir} - R_{red}) / (R_{nir} + R_{red})}$	Bannari et al. (2002)
NDVI	Normalized Difference Vegetation Index	$(R_{nir} - R_{red}) / (R_{nir} + R_{red})$	Rouse et al. (1973)

Predefined Narrowband Greenness (chlorophyll indices)			
CARI	Chlorophyll Absorption Ratio Index	$(R_{700} 670a - R_{670} + b)/(R_{670}(a^2 + 1)^{0.5})$ $a = (R_{700} - R_{550})/150$, $b = R_{550} - a550$	Kim et al. (1994)
BI	Brightness Index	$(R_{800} + R_{670} + R_{550})/\sqrt{3}$	Liu & Moore (1990)
CI	Colouration Index	$(R_{800} - R_{550})/R_{800}$	Liu & Moore (1990)
CTR	Carter Index	R_{695}/R_{760}	Carter (1994)
Datt99	Datt 99	$(R_{850} - R_{710})/(R_{850} - R_{680})$	Datt (1999)
DVI	Difference Vegetation Index	$R_{800} - R_{670}$	Jordan (1969)
REVI1	Revised Enhanced Vegetation Index 1	$2.5((R_{750} - R_{680})/(R_{750} + 6R_{680} - 7.5R_{475} + 1))$	Huete et al., (2002)
REVI2	Revised Enhanced Vegetation Index 2	$2.5((R_{750} - R_{705})/(R_{750} + 6R_{705} - 7.5R_{450} + 1))$	Huete et al., (2002)
mLAI1	Modified Leaf Area Index 1	$3.618 \times EVI1 - 0.118$	Boegh et al. (2002)
mLAI2	Modified Leaf Area Index 2	$3.618 \times EVI2 - 0.118$	Boegh et al. (2002)
GI	Greenness Index	R_{554}/R_{677}	Zarco-Tejada et al. (2005)
GVI	Greenness Vegetation Index	$(R_{682} - R_{553})/(R_{682} + R_{553})$	Gandia et al. (2004)
gNDVI	Green Normalized Difference Vegetation Index	$(R_{780} - R_{550})/(R_{780} + R_{550})$	Smith et al. (1995)
GRg	Gitelson Ratio Green	$(R_{800}/R_{550}) - 1$	Gitelson et al. (2003)
Macc01	Macciono 2001	$(R_{780} - R_{710})/(R_{780} - R_{680})$	Maccioni et al. (2001)
MCARI	Modified Chlorophyll Absorption Ratio Index	$[(R_{700} - R_{670}) - 0.2(R_{700} - R_{550})](R_{700}/R_{670})$	Daughtry et al. (2000)
MCARI2	Modified Chlorophyll Absorption Ratio Index	$1.2[2.5(R_{800} - R_{670}) - 1.3(R_{800} - R_{550})]$	Haboudane et al. (2004)
RMCARI	Revised Modified Chlorophyll Absorption Ratio Index	$[(R_{770} - R_{705}) - 0.2(R_{750} - R_{550})](R_{750}/R_{705})$	Wu et al. (2008)
McM_94	McMurtney	R_{700}/R_{670}	McMurtney et al. (1994)
MRENDVI	Modified Red Edge Normalized Difference Vegetation Index	$(R_{750} - R_{705})/(R_{750} + R_{705} - 2R_{445})$	Datt (2002)
MRESR	Modified Red Edge Simple Ratio	$(R_{750} - R_{445})/(R_{705} + R_{445})$	Sims and Gamon (2002)
MSR	Modified Simple Ratio	$((R_{800}/R_{670}) - 1)/\sqrt{(R_{800}/R_{670}) + 1}$	Chen (1996a)
MSR2	Modified Simple Ratio - Revised	$((R_{750}/R_{705}) - 1)/\sqrt{(R_{750}/R_{705}) + 1}$	Wu et al. (2008)
mTVI	Modified Triangular Vegetation Index	$1.2[1.2(R_{800} - R_{550}) - 2.5(R_{670} - R_{550})]$	Haboudane et al. (2004)

mTVI2	Modified Triangular Vegetation Index - Improved	$\frac{1.5[1.2(R_{800} - R_{550}) - 2.5(R_{670} - R_{550})]}{\sqrt{(2 \times R_{800} + 1)^2 - (6 * R_{800} - 5 \times \sqrt{R_{670}}) - 0.5}}$	Haboudane et al. (2004)
mNDVI1	Modified Normalized Difference Vegetation Index 1	$(R_{800} - R_{680}) / (R_{800} + R_{680} - 2R_{445})$	Sims & Gamon (2002)
mNDVI2	Modified Normalized Difference Vegetation Index 2	$(R_{750} - R_{705}) / (R_{750} + R_{705} - 2R_{445})$	Sims & Gamon (2002)
mNDVI3	Modified Normalized Difference Vegetation Index 3	$(R_{750} - R_{445}) / (R_{750} + R_{705} - 2R_{445})$	Sims & Gamon (2002)
MSAVI	Modified Soil Adjusted Vegetation Index	$0.5 \left[2R_{800} + 1 - \sqrt{(2 \times R_{800} + 1)^2 - 8(R_{800} - R_{670})} \right]$	Qi et al. (1994)
MSR3	Modified Simple Ratio	$(R_{800} - R_{445}) / (R_{680} - R_{445})$	Sims & Gamon (2002)
MSR4	Modified Simple Ratio	$(R_{750} - R_{445}) / (R_{705} - R_{445})$	Sims & Gamon (2002)
MTCI	MERIS Terrestrial Chlorophyll Index	$(R_{754} - R_{709}) / (R_{709} - R_{681})$	Dash & Curran (2004)
NDVI	Normalized Difference Vegetation Index	$(R_{800} - R_{680}) / (R_{800} + R_{680})$	Rouse et al. (1973)
NDVI1	Normalized Difference Vegetation Index 1	$(R_{800} - R_{670}) / (R_{800} + R_{670})$	Tucker (1979)
NDVI2	Normalized Difference Vegetation Index 2	$(R_{750} - R_{705}) / (R_{750} + R_{705})$	Gitelson & Merzlyak (1994)
NDVI3	Normalized Difference Vegetation Index 3	$(R_{755} - R_{745}) / (R_{755} + R_{745})$	Mutanga & Skidmore (2004b)
NDVI4	Normalized Difference Vegetation Index 4	$(R_{755} - R_{730}) / (R_{755} + R_{730})$	Mutanga & Skidmore (2004b)
NDVI5	Normalized Difference Vegetation Index 5	$(R_{700} - R_{670}) / (R_{700} + R_{670})$	Gitelson et al. (2002a)
OSAVI	Optimized Soil Adjusted Vegetation Index	$1.16(R_{800} - R_{670}) / (R_{800} + R_{670} + 0.16)$	Rondeaux et al. (1996)
ROSAVI	Revised Optimized Soil Adjusted Vegetation Index	$1.16(R_{750} - R_{705}) / (R_{750} + R_{705} + 0.16)$	Wu et al. (2008)
RDVI	Renormalized Difference Vegetation Index	$(R_{800} - R_{670}) / \sqrt{R_{800} + R_{670}}$	Roujean & Breon (1995)
REIP	Red Edge Inflection Point	$700 + 40 [(R_{670} + R_{780}) / 2] - R_{700} / (R_{740} - R_{700})$	Guyot & Baret (1988)
Rre	Reflectance at the Inflection Point	$(R_{670} - R_{780}) / 2$	Guyot & Baret (1988)
SIP11	Structure Insensitive Pigment Index 1	$(R_{800} - R_{450}) / (R_{800} - R_{650})$	Panuelas et al. (1995)

SIPI2	Structure Insensitive Pigment Index 2	$(R_{800} - R_{440})/(R_{800} - R_{680})$	Panuelas et al. (1995)
SIPI3	Structure Insensitive Pigment Index 3	$(R_{800} - R_{445})/(R_{800} - R_{680})$	Panuelas et al. (1995)
SIPI4	Structure Insensitive Pigment Index 4	$(R_{800} - R_{455})/(R_{800} - R_{680})$	Panuelas et al. (1995)
SIPI5	Structure Insensitive Pigment Index 5	$(R_{800} - R_{455})/(R_{800} - R_{705})$	Panuelas et al. (1995)
SPVI	Spectral Polygon Vegetation Index	$0.4[3.7(R_{800} - R_{670}) - 1.2(R_{530} - R_{670})]$	Vincini et al. (2006)
PSSRa	Pigment Specific Simple Ratio Chl a	R_{800}/R_{670}	Blackburn (1998b)
PSSRb	Simple Ratio (Also, Pigment Specific Simple Ratio Chl b)	R_{800}/R_{635}	Blackburn (1998b)
SR	Simple Ratio	R_{800}/R_{680}	Jordan (1969)
SR1	Simple Ratio	R_{750}/R_{700}	Gitelson & Merzlyak (1997)
SR2	Simple Ratio	R_{752}/R_{690}	Gitelson & Merzlyak (1997)
SR3	Simple Ratio	R_{750}/R_{550}	Gitelson & Merzlyak (1997)
SR4	Simple Ratio	R_{672}/R_{550}	Datt (1998)
SR5g	Simple Ratio 5	R_{750}/R_{710}	Zarco-Tejada et al. (2001)
TCARI	Transformed Chlorophyll Absorption Ratio Index	$3[(R_{700} - R_{670}) - 0.2(R_{700} - R_{550})(R_{700}/R_{670})]$	Haboudane et al. (2002)
RTCARI	Revised Transformed Chlorophyll Absorption Ratio Index	$3[(R_{750} - R_{705}) - 0.2(R_{750} - R_{550})(R_{750}/R_{705})]$	Wu et al. (2008)
TSAVI	Transformed Solid Adjusted Vegetation Index	$a(R_{875} - aR_{670} - b)/[R_{680} + a(R_{875} - b) + 0.08(1 + a^2)]$ $a = 1.062, b = 0.022$	Rondeaux et al. (1996)
TVI	Triangular Vegetation Index	$0.5[120(R_{750} - R_{550}) - 200(R_{670} - R_{550})]$	Broge & Leblanc (2001)
mVARI1	Modified Visible Atmospherically Resistant Index 1	$(R_{550} - R_{650})/(R_{550} + R_{650} - R_{450})$	Gitelson et al. (2002a); Proposed here
VOG1	Vogelmann Index	R_{740}/R_{720}	Vogelmann et al. (1993)
RTCARI/ROSAVI	(705, 750)	$\frac{3[(R_{750} - R_{705}) - 0.2(R_{750} - R_{550})(R_{750}/R_{705})]}{1.16(R_{750} - R_{705})/R_{750} + R_{705} + 0.16}$	Wu et al. (2008)
RMCARI/ROSAVI	Revised (705, 750)	$\frac{[(R_{750} - R_{705}) - 0.2(R_{750} - R_{550})(R_{750}/R_{705})]}{1.16(R_{750} - R_{705})/R_{750} + R_{705} + 0.16}$	Wu et al. (2008)
<i>Predefined Leaf Pigments (Carotenoids, Anthocyanins)</i>			
ARI1	Anthocyanin Reflectance Index 1	$(1/R_{550}) - (1/R_{700})$	Gitelson et al. (2001)
ARI2	Anthocyanin Reflectance Index 2	$R_{800}[(1/R_{550}) - (1/R_{700})]$	Gitelson et al. (2001)
BGI	Blue Green Pigment Index	R_{450}/R_{550}	Zarco-Tejada et al. (2005)
BRI	Blue Red Pigment Index	R_{450}/R_{690}	Zarco-Tejada et al. (2005)

CRI1	Carotenoid Reflectance Index 1	$(1/R_{510}) - (1/R_{550})$	Gitelson et al. (2002b)
CRI2	Carotenoid Reflectance Index 2	$(1/R_{510}) - (1/R_{700})$	Gitelson et al. (2002b)
mCRI	Modified Carotenoid Reflectance Index	$(1/R_{510} - 1/R_{550}) \times R_{750}$	Gitelson et al. (2006)
RGI	Red Green	R_{690}/R_{550}	Zarco-Tejada et al. (2005)
<i>Predefined Plant Stress/Senescence/Water</i>			
CUR	Curvature Index	$(R_{675} \times R_{690})/R_{683}^2$	Zarco-Tejada et al. (2001, 2003)
LIC	Lichtenthaler	R_{440}/R_{690}	Lichtenthaler et al. (1996)
NPCI	Normalized Pigment Chlorophyll Index	$(R_{680} - R_{430})/(R_{680} + R_{430})$	Panuelas et al. (1994)
NPQI	Normalized Phaeophytinization Index	$(R_{415} - R_{435})/(R_{415} + R_{435})$	Barnes et al. (1992)
PRI	Photochemical Reflectance Index	$(R_{531} - R_{570})/(R_{531} + R_{570})$	Gamon et al. (1997)
PRI2	Photochemical Reflectance Index	$(R_{570} - R_{539})/(R_{570} + R_{539})$	Filella et al. (1996)
PSRI	Plant Senescence Reflectance Index	$(R_{680} - R_{500})/R_{750}$	Merzlyak et al. (1999)
SR5s	Simple Ratio	R_{690}/R_{655}	Zarco-Tejada et al. (2003b)
SR6	Simple Ratio	R_{685}/R_{655}	Zarco-Tejada et al. (2003b)
SRPI	Simple Ratio Pigment Index	R_{430}/R_{680}	Panuelas et al. (1995)
WI	Water Index	R_{970}/R_{900}	Panuelas et al. (1993)

5.2.3.2. Non-parametric multi-variate regression: Gaussian Processes Regression

The GPR Band Analysis Tool (GPR-BAT) algorithm (Chapter 2, Section 2.2.2.) was implemented to analyze the spectral datasets for the five sites described above (i.e. the full spectral dataset and spatial and spectral subsets). The spectral data were processed systematically to assess: (1) the overall performance of the GPR algorithm, measured in terms of r^2 and RMSE for predicting LCC, PAI_e, and CCC_e at the various view zenith angles, spatial scales, and field sites, (2) the optimal wavelength regions for the field variables in question (LCC, PAI_e, and CCC_e) across the various view zenith angles, spatial scales, and field site, and (3) if a given spectral subset (i.e. CHRIS/PROBA Mode-1) was capable of outperforming the full spectrum dataset. For the

full ASD reflectance dataset, the GPR algorithm was programmed to remove 100 bands in each iteration (GPR-100); trials using single band removal per iteration proved to be too lengthy. However, for the CHRIS/PROBA Mode-1 spectral subset one band at a time (GPR-1) was removed since there were only 62 bands in total. All model outputs described above are presented and discussed. The NRMSE was later computed to compare the overall GPR model predictions for the individual and combined variables (i.e. LCC, PAI_e, CCC_e) at the various VZAs. Finally, all modelled prediction results (SR, ROSAVI, and GPR) were ultimately compared using the NRMSE to assess model accuracy

The GPR-BAT algorithm provides the following outputs (see Verrelst et al., 2016): (1) goodness-of-fit validation statistics (e.g. r^2 and RMSE) as a function of number of bands plotted over the sequentially removed bands until one is left (validation statistics are provided for each step with x number of bands), (2) associated wavelengths for each GPR model step, (3) if k -fold cross-validation sub-sampling is applied, then it also provides a frequency of most relative bands (e.g. top 10) for a given number of bands (e.g. all bands) and a list of the best predictor variables (i.e. bands), and (4) sum of the l_b hyperparameter values for all bands in the dataset, where lower values provide an indication of higher predictive power of a spectral band.

5.2.3.3. *Validation: k-fold cross validation*

Validation of the parametric and non-parametric regression modelling was based upon k -fold cross-validation (Snee, 1977). This technique operates by randomly dividing the modelling dataset into equal-sized k sub-datasets (k is defined by the analyst) from which $k-1$ sub-datasets are chosen for training and a single k sub-dataset is chosen for validation. The process is repeated k -times, with each of the k sub-datasets used as a validation dataset. The final step takes the mean score from each validation step to produce a single estimate. The benefit of using k -fold cross-validation

is that all data are used for both training and validation (Verrelst et al., 2015a,b; Verrelst et al., 2016). Cross-validation procedures, specifically k -fold cross-validation, have been used in previous remote sensing studies where parametric and non-parametric models were developed (e.g. Ji et al., 2012; Peng et al., 2017; Verrelst et al., 2015a,b; Verrelst et al., 2016). A significant benefit of k -fold cross-validation is that it can be used with small sample sizes. In this study, a 10-fold ($k=10$) cross-validation procedure was implemented in the ARTMO software package (Verrelst et al., 2012c; Rivera et al., 2014a,b). All model evaluation metrics (r^2 , RMSE, NRMSE) correspond to the k -fold cross-validation procedure and are thus denoted as such (e.g. r^2_{cv} , $RMSE_{cv}$, $NRMSE_{cv}$).

5.2.3.4. ARTMO modelling and retrieval

Parametric and non-parametric empirical modelling was conducted using the Automated Radiative Transfer Models Operator (ARTMO) (Verrelst et al., 2012c) software package, which includes the following: (1) leaf and canopy radiative transfer models (RTMs), including PROSAIL, (2) a spectral indices toolbox, (Rivera et al., 2014b), and (3) a machine learning regression algorithm toolbox (MLRA) (Rivera et al., 2014a; Verrelst et al., 2015; Verrelst et al., 2016). The ARTMO package runs in MATLAB (MathWorks, Inc., Natick, MA, USA) and can be downloaded from <http://ipl.uv.es/artmo/>.

5.3. Results

5.3.1. Field reflectance measurements: Observed differences based on wavelength and view angle

The multi-angle ASD reflectance spectra and associated coefficient of variation values for the various field sites are presented in Figure 39. Since similar studies have characterized Arctic tundra reflectance based on stratification of ground moisture, pH (potential of hydrogen), and plant community composition (Liu et al, 2017; Buchhorn et al., 2013; Bratsch et al., 2016), the focus here is on describing the generalized reflectance anisotropy based on the overall mean reflectance values measured across each field site and view zenith angle. The following sections provide brief descriptions related to: (1) the visible wavelength region (VIS, 400-690 nm), (2) the red-edge slope wavelength region (RE, ~690-750 nm), and (3) the near-infrared wavelength region (NIR, 720-1050 nm) studies (Liu et al, 2017).

In the VIS region, all sites showed an overall trend of increasing reflectance progressing from 330 nm to 690 nm, such as those reported in other Arctic field-based spectroscopy studies (Liu et al, 2017; Buchhorn et al., 2013; Bratsch et al., 2016). This overall increase in the VIS was especially visible for the high Arctic site (Banks Island) where a significant amount of dry bare soil and senescent vegetation occurred in many of the field plots. Sites at lower latitudes had significant proportions of senescent vegetation but displayed an overall lesser degree of visible soil and substrates, based on measurements of PAI_e and associated gap fractions (e.g. Chapter 4). Pigment (chlorophyll) absorption *in situ*, which is centred at approximately 670-680 nm (Gitelson et al., 2004), showed a stronger response in more southerly sites such as the Richardson Mountains, which is explained by a greater overall quantity of chlorophyll and thus vegetation per unit area (i.e. CCC_e). It also had more leaf water content per unit area. The dampened chlorophyll absorption in the red wavelengths observed in this study has also been reported in previous studies (e.g.

Bratsch et al., 2016; Buchhorn et al., 2013; Davidson et al., 2016; Ulrich et al., 2009; Liu et al., 2017). Multi-angle reflectance measurements showed a standard response in the VIS across all sites; i.e. backscattered reflectance at -55° and -36° was greater in all wavelengths than both nadir (0°) and forward scattered measurements at $+55^\circ$ and $+36^\circ$. Nadir and forward scatter reflectance measurements were the most similar. The differences in reflectance spectra between the viewing directions were likely due to combinations of canopy gaps and back-shadow effects (Deering et al., 1999; Sandmeier et al., 1998), and these differences also increased with increasing wavelength. Of note is the coefficient of variation of reflectance values, which tended to decrease with wavelength across all study sites. Generally, reflectance values at lower wavelengths (e.g. ~ 330 nm to ~ 500 nm) showed the highest degree of variability (except for Richardson Mountains 2014), with a pronounced dip in variability at ~ 550 nm (i.e. peak green reflectance), and a subsequent increase in variability at ~ 680 nm (i.e. pigment absorption) at all VZAs. Such a degree of variability may be explained by the sampling gradient employed at each of the field sites (i.e. vegetated to non-vegetated plots). This is especially true for Banks Island where a greater degree of soil backgrounds were sampled (i.e. increased canopy gap fractions). At lower latitude sites, the lower variability of the ~ 550 nm region may be an indication of leaf/canopy carotenoid content (i.e. xanthophylls) in relation to leaf/canopy chlorophyll content, as it has been shown that chlorophyll degrades more rapidly than carotenoids content when plants are undergoing stress or senescence (Merzlyak & Gitelson, 1995; Sims & Gamon, 2002; Croft et al., 2013). Lower variability at ~ 550 may also be an indication of the similar quantity of leaf/canopy carotenoid content found across species/canopy assemblages at each study site. The variability of the ~ 680 nm reflectance signal at sites possessing lower gap fractions (i.e. lower latitude sites) may be an indication of spatial differences between the pigment pools contained within the vegetation

canopies sampled (i.e. different vegetation assemblages/species groupings). Reflectance variability at ~680 observed between similar locations (e.g. Richardson Mountains 2013 and 2014) may be an indication of difference to the time of year sampling was completed; weather (i.e. its influence on plant development, phenology) or the degree of moisture contained within the canopy/soil may impact reflectance in these regions. Variability in relation to VZA showed no clear tendency (i.e. forward and backscatter were both variable across the field sites at all VIS regions). The lower variability observed in the lower VIS region (~330 nm to ~430 nm) of the Richardson Mountains 2014 as compared to the previous field season may be due to the seasonal weather patterns (i.e. plant phenology or moisture) or to the time of year sampling was conducted (phenology/senescence).

For vegetation, the RE region is a transitional zone between low red reflectance related to pigment quantities and leaf water content, and high NIR reflectance related to leaf structure and canopy architecture (e.g. PAI) (leaf water content also plays a role in absorption). The RE is commonly used to estimate LCC and detect vegetation stress (Zarco-Tejada et al., 2003b; Ulrich et al., 2009; Liu et al., 2017). It had the greatest slope at lower latitudes with greater overall quantities of chlorophyll and green leaf matter per unit area (i.e. CCC_e), thus providing a greater difference between red absorption and NIR reflectance as compared to more northerly sites where lower plant matter per unit area results in greater canopy gaps and greater soil and substrate reflectance. The shallowest RE slope was observed in the most northern site (Banks Island, NT). Like the VIS region, greater RE reflectance was observed in the backscatter measurements than in the nadir (0°) and forward scatter measurements. The variability of the RE region is shown in Figure 39. At all field sites and VZAs, RE spectral measurements, showed less variability as compared to the VIS wavelength region; however, the left side of the RE reflectance curve appears

to be affected by the variability observed in the VIS. The lower degree of variability detected in the right wing may be attributable to leaf and canopy structure which will generally have a lower degree of variability after canopy development and during plant stress and/or senescence (i.e. structure is maintained). The coefficient of variation differences between the Richardson Mountains seasons (2013 and 2014) were approximately 0.1 and 0.2, respectively. Difference between these sites may be explained by differences to canopy development between years (i.e. phenology, weather, etc.). No clear trends related to VZA were observed in the RE reflectance variability.

In the NIR wavelength regions, all vegetation plots showed overall low nadir reflectance (<0.5), with the lowest values occurring in the most northern field sites. Similar low reflectance values have been reported in other studies e.g. (<0.4) (Bratsch et al., 2016; Buchhorn et al., 2013; Davidson et al., 2016; Ulrich et al., 2009; Liu et al., 2017), and like other studies, the measurements from this study did not produce the typical NIR reflectance plateau found in green vegetation (e.g. Bratsch et al., 2016; Buchhorn et al., 2013; Davidson et al., 2016; Ulrich et al., 2009; Liu et al., 2017). It has been suggested that the low NIR reflectance could be attributed to low vegetation height/structure and low green leaf area (less multiple backscatter due to lower vertical canopy layering) and a visible understory of moss, lichen, and soil that reduces NIR reflectance (Buchhorn et al., 2013). This was certainly visible in the high Arctic site (Banks Island) where spectra begin to resemble soil reflectance curves. Sites at lower latitudes had a greater proportion of vascular plants per unit area, thereby enhancing the multiple scattering of NIR reflectance (Curran, 1989; Davidson et al., 2016). NIR reflectance was lowest at nadir (0°) for all sites, and as was anticipated, backscatter measurements produced the greatest NIR reflectance followed by forward scatter measurements. The negative backscatter view angles produce the greatest reflectance since

shadows are hidden (Hapke, 1993; Hapke et al., 1996; Breon et al., 2002; Camacho-de Coca et al., 2004). Previous studies have highlighted the importance of NIR reflectance for discriminating vegetation types with different structures, for example sedge dominant vs. moss-dominant (e.g. Bratsch et al., 2016; Buchhorn et al., 2013; Davidson et al., 2016; Ulrich et al., 2009; Liu et al., 2017); however, as shown in the multi-angle measurements below, retrievals are complicated by sun-target-sensor geometry to the point where high NIR values may be due to hotspot effects (reduced or no shadows) and by local topographic slope and aspect variability (i.e. hummocks). Coefficient of variation values for all sites indicate that the lowest reflectance variability exists in this spectral region for all field sites and may be an overall indication of leaf and canopy structure. The observed NIR coefficient of variability for the Richardson Mountains seasons (2013 and 2014) was approximately 0.1 and 0.2, respectively. Such overall differences may be due to the same reasons provided for the lower wavelength spectral regions. No observable trend for the coefficient of variation is observable when examined in the context of VZA.

Figure 39 Averaged field spectra from the various sites and for various look angles (left column). Coefficient of variation for spectral measurements are presented in the right column.

5.3.2. Parametric regression based on vegetation indices (VIs)

Due to the large quantity of results obtained for the VI parametric regression analysis, only an overall summary and the top results for the multi-band and predefined VIs are presented. The full results for the multi-band indices are given in Appendix B and for the predefined indices in Appendix C.

5.3.2.1. Multi-band indices – derivation of the best wavelengths at both spectral and spatial scales

Eleven multi-band VIs were calculated from the field-scale canopy reflectance spectra using all two band combinations (Table 24). In total ~2700 tests were performed (not accounting for the sub-test permutations conducted for finding the optimal cross-validated r^2_{cv} between all spectral bands). Figure 40 (top left) highlights the two-band spectral regions/selections produced from the overall best results for all VIs and all spectral datasets, irrespective of vegetation variable, view angle geometry, spectral subset, investigation scale, or geographic location (all shown). Best band selections were defined as the optimal two-band combinations that produced the highest r^2_{cv} for that VI; no numerical cut-off for r^2_{cv} was used. Although this figure does not show the strength of the relationships, it is apparent that there are specific spectral regions which are of higher importance than others for explaining and predicting LCC, PAI_e, and CCC_e. Figure 40 (top right) shows the same VI test results but coded for VZA (all variables are included). Each figure shows a noticeable clustering of results in the lower VIS wavelengths centred around 350 nm and 550-600 nm, in the RE centred around 700-750 nm and in the NIR around 950 nm to 1075 nm, with noticeable gaps between these regions. Important spectral regions reported here are like those reported by similar ground based studies (e.g. Buchhorn et al., 2013; Liu et al., 2017). Interestingly, many band selections were spectrally near one another (i.e. <10 nm). Figure 40 (bottom left) shows a close-up of the band selections in Figure 40 (top left). Figure 40 (bottom right) shows an ordered frequency distribution of the modelled band differences (i.e. absolute value in nm of Band 2 subtracted from Band 1).

Figure 40 Scatterplots showing band combinations for each variable (top left) and for each angle (top right) over all modes, scales, vegetation variables, or VIs used (full dataset). The Figure on the top left combines all VZAs, whereas the figure on the top right combines all vegetation variables (LCC, PAI_e, and CCC_e). A close-up of the band selections per variable with 1:1 line shown (bottom left). The frequency distribution of the absolute modelled band differences for all multi-band VIs.

When comparing the performance of the VIs across all constraining variables (e.g. VZA, spectral mode/subset, investigation scale/spatial scale, and geographic location), the simple ratio (SR) showed the best combined cross-validated results for explaining all three of the field-based vegetation variables ($r^2_{cv}=0.51$) from the spectral datasets. Overall best results were calculated

from the mean r^2_{cv} values from tests performed across all measurement scenarios (Table 25). It can be assumed that LCC, PAI_e, and CCC_e values were spectrally related (as can be seen in Figure 40, left) and thus one representative VI was selected to explain and predict all three. Table 25 below, presented using a red/white/blue colour ramp to highlight poor (blue gradient, $r^2_{cv}=0.30$) to median (white, $r^2_{cv}=0.45$) to optimal results (red gradient, $r^2_{cv}=0.60$), shows the results of the combined multi-band VIs.

Table 25 Multi-band VIs ranked. Overall ranking based on mean r^2_{cv} and incorporates tests from all variables, angles, scales, and spectral modes (i.e. full spectrum vs. resampled CHRIS Mode-1).

<i>Colour Scale (r^2_{cv})</i>			<i>ASD (Full spectrum)</i>		<i>CHRIS M1 (Spectral subset)</i>	
			<i>Subplot</i>	<i>Plot</i>	<i>Subplot</i>	<i>Plot</i>
<i>VI</i>	<i>Rank</i>	<i>Mean r^2_{cv}</i>	<i>r^2_{cv}</i>	<i>r^2_{cv}</i>	<i>r^2_{cv}</i>	<i>r^2_{cv}</i>
SR	1	0.51	0.48	0.58	0.45	0.53
NDVI	2	0.50	0.47	0.57	0.44	0.53
IPVI	3	0.50	0.46	0.57	0.44	0.53
SRNDVI	4	0.49	0.46	0.54	0.44	0.52
SAVI	5	0.48	0.42	0.58	0.38	0.54
MSR	6	0.47	0.40	0.57	0.40	0.52
MNLI	7	0.47	0.40	0.56	0.38	0.54
RDVI	8	0.47	0.36	0.58	0.38	0.55
DVI	9	0.46	0.41	0.56	0.35	0.52
NLI	10	0.46	0.42	0.50	0.39	0.51
TDVI	11	0.34	0.32	0.33	0.36	0.34

Boxplots of r^2_{cv} for each VI vs each field variable can be seen in Figure 41. What is surprising here is that all tests produced very comparable results, suggesting that the wavelength regions used in a VI are more important than the VI formulation itself. Another important result is that relationships/correlations reported at the plot scale were almost always stronger than those reported at the subplot scale (e.g. Table 25). For instance, SR produced an $r^2_{cv}=0.48$ at the subplot scale and an $r^2_{cv}=0.58$ at the plot scale with the full spectrum ASD dataset; similar differences were observed for the M1 spectral subset. The spatial sampling used in the field suggests that it is important to account for spatial variability when collecting spectra or measuring bio-geophysical

variables in the Arctic, since vegetation canopies are highly variable at the 1 m² scale; accordingly, these results concur with Laidler et al. (2008), showing that measurements should be averaged over larger homogeneous areas when retrieving Arctic biophysical and biochemical variables.

Figure 41 Comparison of multi-band vegetation indices for all look angles, across all sites, all spatial scales, and for all spectral modes (all combined into one dataset). Multi-band VIs arranged by r^2_{cv} (largest (left) to smallest (right)). Boxplots show the interquartile range with factor of 1.5; outliers are displayed with +.

Given that most of the VIs performed quite similarly, SR was selected for further analysis since it is the simplest formulation, it was least affected by view angle geometry and it produced comparable results for LCC, PAI_e , and CCC_e .

5.3.2.2. Simple Ratio (SR) vegetation index: detailed analysis

The full results from the cross-validated SR regression analyses/retrievals can be seen in Table 26. Across all field sites, VZAs, and spectral subsets, SR produced greater r^2_{cv} values and lower $RMSE_{cv}$ at the plot scale than at the subplot scale for LCC, PAI_e , and CCC_e retrievals (significantly different at the $p \leq 0.05$ level); therefore, plot-scale values are discussed here in relation to: (1) vegetation variables, (2) VZAs, (3) spectral subsets, and (4) geographic locations. Because of the number of testing conditions, the results are too numerous to fully discuss. Tables are presented using a colour ramp from blue ($r^2_{cv}=0$) through red ($r^2_{cv}=1$). All results are presented with their associated error metrics ($RMSE_{cv}$).

Table 26 Results for Simple Ratio (SR) multi-band vegetation index. r^2_{cv} values are colour coded on a continuous scale: blue = low r^2_{cv} values (0.0) and red = high r^2_{cv} values (1.0). Plotted relationships (scatterplots) are bolded and marked with an asterisk.

Colour Scale (r^2_{cv})			ASD (Full spectrum)				CHRIS M1 (Spectral subset)			
0 1			Subplot		Plot		Subplot		Plot	
Location	VZA	Variable	r^2_{cv}	$RMSE_{cv}$	r^2_{cv}	$RMSE_{cv}$	r^2_{cv}	$RMSE_{cv}$	r^2_{cv}	$RMSE_{cv}$
Herschel	0°	LCC*	0.21	6.14	0.66	3.08	0.20	6.17	0.69	3.29
Island		PAI_e	0.16	0.30	0.61	0.19	0.14	0.30	0.63	0.19
(2011)		CCC_e	0.27	0.12	0.62	0.06	0.27	0.12	0.70	0.06
Banks	0°	LCC	0.60	7.29	0.78	3.45	0.59	7.03	0.76	3.45
Island		PAI_e	0.56	0.20	0.85	0.07	0.60	0.17	0.85	0.08
(2012)		CCC_e	0.59	0.07	0.72	0.04	0.65	0.07	0.75	0.04
	-36°	LCC	0.71	6.51	0.70	3.82	0.70	6.60	0.72	3.96
		PAI_e	0.65	0.18	0.91	0.07	0.65	0.18	0.91	0.07
		CCC_e	0.66	0.06	0.88	0.03	0.66	0.06	0.88	0.03
	-55°	LCC	0.69	6.66	0.74	3.88	0.69	6.70	0.74	3.91
		PAI_e	0.68	0.18	0.87	0.08	0.68	0.18	0.88	0.08
		CCC_e	0.64	0.06	0.81	0.04	0.64	0.06	0.82	0.04
	+36°	LCC	0.63	8.07	0.68	3.93	0.60	8.28	0.70	3.83
		PAI_e	0.56	0.19	0.94	0.09	0.56	0.19	0.91	0.09
		CCC_e *	0.72	0.06	0.96	0.03	0.72	0.06	0.93	0.03
	+55°	LCC	0.65	7.14	0.64	3.83	0.64	7.27	0.65	3.86
		PAI_e	0.57	0.21	0.83	0.11	0.55	0.21	0.84	0.11
		CCC_e	0.62	0.07	0.82	0.05	0.61	0.07	0.80	0.05

<i>Richards Island (2013)</i>	0°	<i>LCC</i>	0.55	3.64	0.36	3.56	0.59	3.90	0.46	3.58
		<i>PAI_e</i>	0.49	0.14	0.81	0.11	0.49	0.15	0.48	0.18
		<i>CCC_e</i>	0.46	0.07	0.15	0.08	0.48	0.07	0.37	0.08
	-36°	<i>LCC</i>	0.62	4.30	0.41	3.51	0.63	4.50	0.50	4.10
		<i>PAI_e</i>	0.76	0.15	0.63	0.15	0.47	0.18	0.51	0.19
		<i>CCC_e</i>	0.61	0.07	0.60	0.07	0.66	0.08	0.34	0.08
	-55°	<i>LCC</i>	0.32	4.23	0.67	3.44	0.49	4.46	0.38	3.88
		<i>PAI_e *</i>	0.44	0.15	0.78	0.15	0.71	0.15	0.69	0.20
		<i>CCC_e</i>	0.66	0.08	0.42	0.08	0.73	0.08	0.73	0.08
	+36°	<i>LCC</i>	0.54	3.83	0.58	3.40	0.42	4.32	0.27	3.64
		<i>PAI_e</i>	0.65	0.13	0.44	0.18	0.53	0.16	0.18	0.22
		<i>CCC_e</i>	0.59	0.07	0.44	0.07	0.49	0.07	0.18	0.09
	+55°	<i>LCC</i>	0.69	4.01	0.57	3.17	0.61	4.15	0.49	3.44
		<i>PAI_e</i>	0.48	0.13	0.59	0.14	0.49	0.15	0.48	0.17
		<i>CCC_e</i>	0.60	0.07	0.42	0.07	0.55	0.07	0.42	0.07
<i>Richardson Mountains (2013)</i>	0°	<i>LCC</i>	0.32	4.73	0.50	3.69	0.34	4.81	0.36	4.12
		<i>PAI_e</i>	0.49	0.19	0.69	0.12	0.51	0.19	0.66	0.13
		<i>CCC_e</i>	0.34	0.10	0.50	0.07	0.32	0.09	0.55	0.07
	-36°	<i>LCC</i>	0.30	4.84	0.20	4.51	0.20	5.37	0.17	4.83
		<i>PAI_e</i>	0.34	0.21	0.53	0.17	0.36	0.21	0.51	0.17
		<i>CCC_e</i>	0.35	0.10	0.29	0.10	0.19	0.10	0.18	0.10
	-55°	<i>LCC</i>	0.39	5.09	0.41	3.86	0.20	5.25	0.33	4.11
		<i>PAI_e</i>	0.40	0.19	0.33	0.18	0.41	0.20	0.29	0.18
		<i>CCC_e</i>	0.34	0.10	0.47	0.09	0.26	0.10	0.25	0.10
	+36°	<i>LCC</i>	0.35	4.46	0.52	3.88	0.31	4.57	0.30	4.04
		<i>PAI_e</i>	0.48	0.18	0.47	0.15	0.47	0.19	0.47	0.15
		<i>CCC_e</i>	0.26	0.10	0.48	0.09	0.31	0.10	0.48	0.09
	+55°	<i>LCC</i>	0.43	4.68	0.46	3.94	0.25	5.10	0.30	4.39
		<i>PAI_e</i>	0.43	0.20	0.52	0.17	0.56	0.19	0.50	0.16
		<i>CCC_e</i>	0.44	0.09	0.45	0.08	0.43	0.09	0.46	0.09
<i>Richardson Mountains (2014)</i>	0°	<i>LCC</i>	0.29	3.69	0.48	2.09	0.29	3.70	0.39	1.77
		<i>PAI_e</i>	0.44	0.32	0.51	0.29	0.38	0.33	0.39	0.34
		<i>CCC_e</i>	0.37	0.15	0.51	0.13	0.21	0.17	0.45	0.14
	-36°	<i>LCC</i>	0.21	3.78	0.42	1.93	0.20	3.88	0.34	2.00
		<i>PAI_e</i>	0.47	0.31	0.69	0.31	0.47	0.33	0.60	0.33
		<i>CCC_e</i>	0.35	0.16	0.48	0.13	0.23	0.16	0.57	0.15
	-55°	<i>LCC</i>	0.27	3.60	0.45	2.15	0.23	3.67	0.43	2.13
		<i>PAI_e</i>	0.41	0.32	0.49	0.28	0.40	0.32	0.46	0.31
		<i>CCC_e</i>	0.34	0.16	0.52	0.12	0.22	0.16	0.51	0.13
	+36°	<i>LCC</i>	0.28	3.59	0.47	2.03	0.21	3.73	0.47	2.05
		<i>PAI_e</i>	0.47	0.31	0.44	0.31	0.44	0.32	0.40	0.31
		<i>CCC_e</i>	0.43	0.15	0.46	0.13	0.42	0.15	0.39	0.13
	+55°	<i>LCC</i>	0.28	3.86	0.59	2.03	0.10	3.96	0.39	2.02
		<i>PAI_e</i>	0.64	0.28	0.56	0.27	0.48	0.31	0.56	0.27
		<i>CCC_e</i>	0.45	0.15	0.70	0.11	0.50	0.15	0.37	0.12
<i>All Sites</i>	<i>Overall</i>		0.48	-	0.58	-	0.45	-	0.53	-
	<i>All</i>	<i>LCC</i>	0.44	4.96	0.54	3.29	0.40	5.12	0.47	3.45
	<i>All</i>	<i>PAI_e</i>	0.50	0.21	0.64	0.17	0.49	0.22	0.58	0.19
	<i>All</i>	<i>CCC_e</i>	0.48	0.10	0.56	0.08	0.45	0.10	0.53	0.08
	0°	<i>LCC</i>	0.39	5.10	0.56	3.17	0.40	5.12	0.53	3.24
	-36°	<i>LCC</i>	0.46	4.86	0.43	3.44	0.43	5.09	0.43	3.72
	-55°	<i>LCC</i>	0.42	4.90	0.57	3.33	0.40	5.02	0.47	3.51
	+36°	<i>LCC</i>	0.45	4.99	0.56	3.31	0.39	5.23	0.44	3.39

+55°	<i>LCC</i>	0.51	4.92	0.57	3.24	0.40	5.12	0.46	3.43
0°	<i>PAI_e</i>	0.43	0.23	0.69	0.16	0.42	0.23	0.60	0.18
-36°	<i>PAI_e</i>	0.56	0.21	0.69	0.18	0.49	0.23	0.63	0.19
-55°	<i>PAI_e</i>	0.48	0.21	0.62	0.17	0.55	0.21	0.58	0.19
+36°	<i>PAI_e</i>	0.54	0.20	0.57	0.18	0.50	0.22	0.49	0.19
+55°	<i>PAI_e</i>	0.53	0.21	0.63	0.17	0.52	0.22	0.60	0.18
0°	<i>CCC_e</i>	0.41	0.10	0.50	0.08	0.39	0.10	0.56	0.08
-36°	<i>CCC_e</i>	0.49	0.10	0.56	0.08	0.44	0.10	0.49	0.09
-55°	<i>CCC_e</i>	0.50	0.10	0.56	0.08	0.46	0.10	0.58	0.09
+36°	<i>CCC_e</i>	0.50	0.09	0.59	0.08	0.49	0.09	0.50	0.09
+55°	<i>CCC_e</i>	0.53	0.09	0.60	0.08	0.52	0.09	0.51	0.08
0°	<i>All</i>	0.41	-	0.58	-	0.40	-	0.57	-
-36°	<i>All</i>	0.50	-	0.56	-	0.45	-	0.52	-
-55°	<i>All</i>	0.47	-	0.58	-	0.47	-	0.54	-
+36°	<i>All</i>	0.50	-	0.57	-	0.46	-	0.47	-
+55°	<i>All</i>	0.52	-	0.60	-	0.48	-	0.52	-

The SR regression analysis produced overall higher mean r^2_{cv} values for *PAI_e* (r^2_{cv} =0.64, $RMSE_{cv}$ =0.17) than for *LCC* (r^2_{cv} =0.54, $RMSE_{cv}$ =3.29) or *CCC_e* (r^2_{cv} =0.56, $RMSE_{cv}$ =0.08) using the full spectrum dataset, and equally so for the M1 dataset (*LCC*, r^2_{cv} =0.47, $RMSE_{cv}$ =3.45; *PAI_e*, r^2_{cv} =0.58, $RMSE_{cv}$ =0.19; *CCC_e*, r^2_{cv} =0.53, $RMSE_{cv}$ =0.08). Visualization of these results can be seen below in the boxplots (Figure 42). It is likely that *PAI_e* models achieved higher correlations since the easily detectable greenness (i.e. leaf area) of a canopy may not necessarily reflect higher quantities of chlorophyll; i.e. a canopy at the m² scale may exhibit greater detectability vs. pigment quantities at the cm² or finer scales.

Another important result here is that the narrower bands of the ASD dataset produced slightly higher overall accuracies and correlations than the resampled M1 datasets; this is visible at most VZAs (Table 26, Figure 42). Higher r^2_{cv} and $RMSE_{cv}$ values for the narrower bands may be because they more precisely detect changes in reflectance due to narrow vegetation absorption features; however, the bandwidth of the CHRIS M1 spectral dataset (~10 nm bandwidth) should theoretically provide sufficient spectral sensitivity towards the variables under investigation (Figure 42).

The VZA that produced the best mean correlations for all three vegetation variables (inclusive) was $+55^\circ$ (mean $r^2_{cv}=0.60$) for the full ASD dataset; however, mean r^2_{cv} values for each angle were comparable, being within ± 0.04 for all other VZAs.

Figure 42 Cross validated SR r^2_{cv} values across all field sites, angles, and variables (at plot scale). *Herschel Island is the only field location that does not have a multi-angle field dataset.

A noteworthy result of the SR modelling was that the Banks Island (2012) datasets produced substantially better predictions and relationships than all other field locations for all vegetation variables under all measurement conditions (Figure 42, bottom right). Cross-validated r^2_{cv} values were high for all variables (e.g. LCC, $r^2_{cv}=0.78$, $RMSE_{cv}=3.45$; PAI_e , $r^2_{cv}=0.94$, $RMSE_{cv}=0.09$; CCC_e , $r^2_{cv}=0.96$, $RMSE_{cv}=0.03$). All other field sites that were sampled with a multi-angle approach produced substantially poorer results (Figure 42, bottom right). Herschel Island (2011) data produced higher than average results for nadir VZA; this dataset did not include multi-angle sampling. The Richardson Mountains (2013, 2014) and Richards Island (2013) field sites show comparable r^2_{cv} and $RMSE_{cv}$ ranges. The strong results achieved for Banks Island may be due to the large spatial variation in PAI_e values, where sites ranged from almost bare to completely covered with vegetation. All other sites possessed overall greater PAI_e values and showed less spatial heterogeneity with respect to canopy gap fraction (see Chapter 4). Near zero values in the biochemical-biophysical variables help to ground the regression line near zero and produce greater linearity. It is also possible that canopy depth (i.e. canopy height) played a role in the prediction strength. Canopy depths were minimal in the high Arctic (i.e. almost two-dimensional) as compared to those at the lower latitude sites. Greater vertical canopy complexity/height has the potential to obscure elements of the canopy. Scatter plots showing best predictions (measured vs. predicted) are shown below (LCC, Herschel Island 0°; PAI_e , Richards Island -55°; CCC_e ; Banks Island +36°) (Figure 43).

Figure 43 Various cross-validated (cv) predictions of the field variables (LCC, PAI_e, and CCC_e) using the SR vegetation index at the plot scale.

Table 27 shows the band selections for each cross-validated SR regression analysis for the various vegetation variables, field sites, view zenith angles, spectral subsets, and spatial sampling scales. A wide diversity of optimal spectral bands across the full ASD spectral sensitivity range was produced from the various datasets. It is therefore difficult to determine if there are any overall underlying trends to the selection of these bands based on VZA alone. To best interpret the large number of optimal bands across these factors, the globally-optimal bands were calculated using a weighted-mean with the associated r^2_{cv} values as the weights. Optimal weighted mean band selections for LCC at all angles, spectral subsets, spatial subsets, and for all sites was, not surprisingly clustered around the VIS pigment absorption regions for chlorophyll ($B1 = 616\text{-}710$ nm) and within the RE and NIR regions typical of healthy vegetation ($B2 = 797\text{-}881$ nm). LCC also showed the highest degree of variability and range of the three field variables with respect to the selected optimal bands. Optimal weighted bands for PAI_e were centred in the VIS-RE regions ($B1 = 623\text{-}707$ nm; $B2 = 622\text{-}721$ nm), but excluded the NIR. Optimal weighted bands for CCC_e were somewhat longer in wavelength and included VIS, RE and short NIR wavelengths ($B1 = 640\text{-}$

760 nm; B2 = 629-798 nm). Band selections for LCC, PAI_e, and CCC_e match very closely to those reported in other studies that have measured similar green vegetation variables, such as percent vegetation cover (~680-872 nm) (Liu et al., 2017) and biomass quantity (~680-872 nm) (Buchhorn et al., 2013).

Table 27 Band selections (B1 and B2) for cross-validated SR regressions. Weighted mean centre of the spectral space is presented as the optimal bands for predicting the field variables. Weighting was calculated using the r^2_{cv} values from the associated cross validated test results.

			<i>ASD (Full spectrum)</i>				<i>CHRIS M1 (Spectral subset)</i>			
			<i>Subplot</i>		<i>Plot</i>		<i>Subplot</i>		<i>Plot</i>	
<i>Location</i>	<i>VZA</i>	<i>Variable</i>	<i>B1</i>	<i>B2</i>	<i>B1</i>	<i>B2</i>	<i>B1</i>	<i>B2</i>	<i>B1</i>	<i>B2</i>
<i>Herschel Island (2011)</i>	0°	<i>LCC</i>	511	512	511	512	510	520	500	520
		<i>PAI_e</i>	531	532	577	576	520	551	661	561
		<i>CCC_e</i>	474	542	965	928	471	540	510	530
<i>Banks Island (2012)</i>	0°	<i>LCC</i>	364	1063	700	883	411	748	697	886
		<i>PAI_e</i>	964	710	711	537	728	540	709	540
		<i>CCC_e</i>	1047	338	716	715	530	551	716	722
	-36°	<i>LCC</i>	373	1048	337	812	411	877	411	915
		<i>PAI_e</i>	750	722	515	570	748	722	510	572
		<i>CCC_e</i>	727	724	567	519	728	722	540	520
	-55°	<i>LCC</i>	400	1048	337	940	411	925	411	940
		<i>PAI_e</i>	740	716	401	565	742	716	411	561
		<i>CCC_e</i>	418	550	399	528	411	551	411	530
	+36°	<i>LCC</i>	351	943	355	752	411	940	411	808
		<i>PAI_e</i>	730	769	582	575	728	770	722	520
		<i>CCC_e</i>	426	550	582	575	442	551	581	572
	+55°	<i>LCC</i>	343	941	608	936	411	940	672	940
		<i>PAI_e</i>	743	744	699	694	722	748	703	691
		<i>CCC_e</i>	515	542	583	572	510	540	581	572
<i>Richards Island (2013)</i>	0°	<i>LCC</i>	1004	967	987	998	777	762	987	997
		<i>PAI_e</i>	969	980	921	922	965	997	925	915
		<i>CCC_e</i>	980	969	978	969	965	997	925	915
	-36°	<i>LCC</i>	997	996	998	1034	561	540	905	940
		<i>PAI_e</i>	600	606	1049	1045	590	603	510	500
		<i>CCC_e</i>	956	958	992	1036	925	987	540	411
	-55°	<i>LCC</i>	347	349	1000	1007	471	411	987	965
		<i>PAI_e</i>	338	340	604	606	590	603	613	603
		<i>CCC_e</i>	401	400	906	907	603	590	613	603
	+36°	<i>LCC</i>	773	772	380	382	777	770	965	997
		<i>PAI_e</i>	391	398	925	926	976	987	965	987
		<i>CCC_e</i>	984	981	925	926	987	976	987	965
	+55°	<i>LCC</i>	977	996	960	992	976	997	965	997
		<i>PAI_e</i>	986	974	988	973	748	755	755	762
		<i>CCC_e</i>	995	991	748	765	976	997	748	762
<i>Richardson Mountains (2013)</i>	0°	<i>LCC</i>	734	733	1027	1043	742	722	735	742
		<i>PAI_e</i>	632	457	676	681	631	461	697	461
		<i>CCC_e</i>	974	972	673	682	510	461	915	572

<i>Richardson Mountains (2014)</i>	-36°	<i>LCC</i>	1021	1019	1028	1030	905	925	886	976
		<i>PAI_e</i>	507	456	578	701	510	452	572	703
		<i>CCC_e</i>	470	469	475	474	500	461	461	500
	-55°	<i>LCC</i>	362	360	976	819	987	777	987	808
		<i>PAI_e</i>	404	403	504	467	500	471	500	471
		<i>CCC_e</i>	475	474	981	980	500	461	481	471
	$+36^\circ$	<i>LCC</i>	837	953	953	931	841	955	955	868
		<i>PAI_e</i>	701	456	456	538	703	452	452	540
		<i>CCC_e</i>	1008	1010	752	750	500	461	755	742
	$+55^\circ$	<i>LCC</i>	1031	1029	1029	1031	976	785	895	976
		<i>PAI_e</i>	410	405	962	1019	622	452	452	603
		<i>CCC_e</i>	1042	1018	1044	1019	510	471	551	452
	0°	<i>LCC</i>	708	969	620	424	703	965	770	572
		<i>PAI_e</i>	543	557	1048	924	540	551	716	987
		<i>CCC_e</i>	716	1050	1048	925	716	976	716	987
	-36°	<i>LCC</i>	450	339	798	805	770	808	800	808
		<i>PAI_e</i>	544	557	497	498	540	561	490	500
		<i>CCC_e</i>	377	366	1057	1055	530	561	490	500
	-55°	<i>LCC</i>	867	862	739	755	868	859	742	755
		<i>PAI_e</i>	544	557	1019	1043	540	561	490	500
		<i>CCC_e</i>	1043	1019	1019	1043	490	500	722	755
	$+36^\circ$	<i>LCC</i>	423	421	581	412	452	411	581	411
		<i>PAI_e</i>	717	1007	722	956	716	997	722	955
		<i>CCC_e</i>	713	956	721	956	716	955	722	955
	$+55^\circ$	<i>LCC</i>	1027	992	352	447	561	748	808	785
		<i>PAI_e</i>	1039	1040	762	737	540	561	762	735
		<i>CCC_e</i>	736	765	585	1063	709	770	997	603
<i>All sites</i>	<i>Overall</i>		685	750	718	770	648	708	655	687
	<i>All</i>	<i>LCC</i>	648	881	685	798	616	797	710	832
	<i>All</i>	<i>PAI_e</i>	675	654	707	721	676	653	623	623
	<i>All</i>	<i>CCC_e</i>	730	729	760	798	647	689	640	629
	0°	<i>LCC</i>	669	910	737	759	626	756	712	745
	-36°	<i>LCC</i>	698	945	685	888	564	752	677	907
	-55°	<i>LCC</i>	456	723	728	901	566	741	704	880
	$+36^\circ$	<i>LCC</i>	583	812	547	627	603	825	637	740
	$+55^\circ$	<i>LCC</i>	794	985	716	842	724	926	816	928
	0°	<i>PAI_e</i>	770	669	779	719	712	629	732	645
	-36°	<i>PAI_e</i>	618	607	644	686	616	605	518	567
	-55°	<i>PAI_e</i>	537	532	601	660	611	606	498	550
	$+36^\circ$	<i>PAI_e</i>	619	640	649	708	785	803	680	656
	$+55^\circ$	<i>PAI_e</i>	820	817	836	837	659	627	675	697
	0°	<i>CCC_e</i>	883	744	853	819	647	692	731	713
	-36°	<i>CCC_e</i>	690	688	773	765	752	773	518	494
	-55°	<i>CCC_e</i>	529	567	763	816	509	548	551	596
	$+36^\circ$	<i>CCC_e</i>	728	824	709	752	648	731	688	724
	$+55^\circ$	<i>CCC_e</i>	809	816	699	834	680	701	684	590
	0°	<i>All</i>	775	771	787	761	663	691	725	699
	-36°	<i>All</i>	666	736	698	764	643	706	562	638
	-55°	<i>All</i>	510	602	694	788	565	625	576	662
	$+36^\circ$	<i>All</i>	645	754	636	696	686	784	669	706
	$+55^\circ$	<i>All</i>	808	872	752	838	685	737	719	729

To provide a better visualization of optimal band selections within their associated spectral space, two-band selections were graphed with their accompanying r^2_{cv} value (Figure 44). Surface-map visualizations such as these allow for a qualitative interpretation of spectral space and an assessment of the optimal regions that are of greater importance to the variable in question. These maps are not plotted using the weighted mean of the spectral space, but highlight the same spectrally important regions. In Figure 44, all variables demonstrated a high degree of spectral variability with respect to VZA; however, several patterns are evident as optimal spectral regions are generally quite distinct from other regions in this Figure. For LCC, there appear to be two distinct large spectral regions that produce above average results for all VZAs that are centred within B1~350-550 nm and B2~700-950 nm. PAI_e and CCC_e, on the other hand, appear to have very defined small optimal spectral areas that vary slightly with VZA. Using the weighted averages to examine wavelength position with VZA, it can be shown that there is in fact a spectral shift that occurs with VZA when predicting LCC, PAI_e, and CCC_e. Figure 45 demonstrates that at negative view angles (i.e. backscatter) shorter wavelengths are optimal as compared to longer wavelengths at positive view angles (i.e. forward scatter). The averaged spectral shift appears to be on the order of 100 nm when progressing from -55° to +55° (the former being when the average sun position is approximately equivalent with the negative sensor angle). All two-band combinations appeared to co-vary with each other and show similar increases in their wavelengths. However, the amount of variability observed in the band selections (Figure 45) may also be the result of chance (natural variability) or noise/error encountered in the measured spectroscopic signals. This seems like an obvious conclusion considering that reflectance magnitude increases or decreases across the sampled VZAs (Figure 39). Observed peaks at the 0° VZA and subsequent dip at the +36° VZA are observable for all variables; reasons for this are not understood.

Figure 44 All 2-band optimal variable selections for the simple ratio (x and y axes) and their associated r^2_{cv} values (z-axis) for each of the view angles (at plot scale, not weighted). One or more distinct optimal spectral regions for each field variable and VZA are evident in each graph.

Figure 45 Weighted band selections for each vegetation variable and view zenith angle for SR VI. Optimal bands selected in the SR optimization show that wavelength selections increase generally from backscatter to forward scatter, where PAI_e shows the best example of this.

5.3.2.3. Predefined narrowband vegetation indices

A total of 84 predefined VIs (Table 24) were examined with the four field-scale reflectance datasets. In total, ~20,000 (VI x view angle x variable x spectral dataset x spatial scale) tests were performed. Figure 46 shows the combined performance (r^2_{cv}) of each predefined narrowband VI for LCC, PAI_e, and CCC_e across all the above factors.

Figure 46 Overall results of the pre-defined narrowband vegetation index modelling based on average r^2_{cv} value from all test variables (i.e. vegetation variables, spectral modes, scales of investigation, and locations). VIs are ordered from higher average r^2_{cv} (left) to lower (right).

The overall top ten performing predefined VIs are shown below in Table 28 (for each spectral subset and plot/subplot scale, but averaged over all angles and field variables) and in Figure 47 (for each field variable but averaged over all angles, spectral datasets and plot/subplot scales). These rankings were not assessed for statistically significant differences; the differences between proximally ranked VIs are probably not significant. The best overall VI was the Revised Optimized Soil Adjusted Vegetation Index (ROSAVI) (Wu et al., 2008), which produced an average $r^2_{cv}=0.36$ at the subplot scale and $r^2_{cv}=0.55$ at the plot scale (for both the full ASD and CHRIS simulated M1 spectral modes) and a global mean of approximately $r^2_{cv}=0.45$ (Figure 46). The Blue Green Index (BGI) (Zarco-Tejada et al., 2005) produced almost identical results to ROSAVI. Other notable

high performing VIs were, as for ROSAVI, based on the Soil Adjusted Vegetation Index (SAVI) (Huete, 1988), such as OSAVI (Rondeau, 1996), TSAVI (Baret & Guyot, 1991), and RMCARI (Wu et al., 2008), which is not surprising given the sparse nature of Arctic tundra vegetation canopies.

It should be noted that the 10 nm bandwidth M1 bands were chosen to match the CHRIS bands and therefore often did not match the central wavelength of a given VI perfectly (e.g. 705/750 ROSAVI vs. 703/748 nm for CHRIS M1). However, both ASD and simulated M1 data produced almost identical results. All results showed moderate strength relationships of the pre-defined narrowband VIs with LCC, PAI_e, and CCC_e at the plot scale that are close to those presented for the multi-band SR assessment. Also, similar to the previous VI optimal band selection analysis, it is evident in Figure 46 that variability is high and that there are no significant differences between the top 10-20 (at least) narrowband VIs. Thus, the choice of ROSAVI for further analysis was arbitrarily based on the best set of mean r^2_{cv} values as shown in Table 28, which are presented using a red/white/blue colour ramp to highlight poor (blue gradient, $r^2_{cv}=0.30$) to median (white, $r^2_{cv}=0.45$) to optimal results (red gradient, $r^2_{cv}=0.60$).

Table 28 Top ten narrowband VIs. Overall ranking based on r^2_{cv} and incorporates tests from all variables, angles, scales, and spectral modes. The top ten narrowband VIs performed quite similarly to each other. 4 decimal places are displayed to show subtle but non-significant differences.

<i>Colour Scale (r^2_{cv})</i>			<i>ASD (Full spectrum)</i>		<i>CHRIS M1 (spectral subset)</i>	
			<i>Subplot</i>	<i>Plot</i>	<i>Subplot</i>	<i>Plot</i>
<i>VI</i>	<i>Rank</i>	<i>Mean</i>	r^2_{cv}	r^2_{cv}	r^2_{cv}	r^2_{cv}
ROSAVI	1	0.4470	0.3580	0.5361	0.3587	0.5354
<i>BGI</i>	<i>2</i>	<i>0.4469</i>	<i>0.3465</i>	<i>0.5461</i>	<i>0.3474</i>	<i>0.5475</i>
<i>NDVI2</i>	<i>3</i>	<i>0.4444</i>	<i>0.3653</i>	<i>0.5233</i>	<i>0.3642</i>	<i>0.5247</i>
<i>CTR</i>	<i>4</i>	<i>0.4400</i>	<i>0.3571</i>	<i>0.5209</i>	<i>0.3566</i>	<i>0.5253</i>
<i>REVI2</i>	<i>5</i>	<i>0.4364</i>	<i>0.3502</i>	<i>0.5211</i>	<i>0.3547</i>	<i>0.5195</i>
<i>OSAVI</i>	<i>6</i>	<i>0.4363</i>	<i>0.3481</i>	<i>0.528</i>	<i>0.3431</i>	<i>0.5262</i>
<i>TSAVI</i>	<i>7</i>	<i>0.4361</i>	<i>0.3467</i>	<i>0.5267</i>	<i>0.3467</i>	<i>0.5245</i>
<i>mLAI2</i>	<i>8</i>	<i>0.4324</i>	<i>0.3447</i>	<i>0.5211</i>	<i>0.3442</i>	<i>0.5195</i>
<i>SRI</i>	<i>9</i>	<i>0.4338</i>	<i>0.3513</i>	<i>0.5155</i>	<i>0.3475</i>	<i>0.5209</i>
<i>RMCARI/ROSAVI</i>	<i>10</i>	<i>0.4336</i>	<i>0.3595</i>	<i>0.5092</i>	<i>0.3577</i>	<i>0.5081</i>

Figure 47 The ten overall best narrowband indices (average r^2_{cv}) shown for each of the vegetation variables (LCC, PAI_e , CCC_e) averaged across all view angles, spectral datasets (ASD and M1), and spatial scales (subplot and plot).

5.3.2.4. Revised Optimized Soil Adjusted Vegetation Index (ROSAVI): detailed analysis

The formulation of ROSAVI (Wu et al., 2008) uses wavelengths centred around 705 and 750 nm. ROSAVI is based on OSAVI (Rondeaux et al., 1996), which was designed to reduce the sensitivity towards background materials, and particularly, underlying soil reflectance properties (Wu et al., 2008). OSAVI was in turn based upon the Soil Adjusted Vegetation Index (SAVI) (Huete, 1988). Since many VIs are influenced by background materials, such as underlying soil and leaf litter, OSAVI has been integrated with other spectral indices to reduce this effect, producing VIs such as ROSAVI, TCARI, and MCARI (Table 24). In a study conducted by Wu et al. (2008), sensitivity tests showed that ROSAVI has overall better linearity with chlorophyll content and resistance to leaf area index variations by considering the effect of quick saturation at 670 nm with relatively low chlorophyll content. The full plot scale results of the ROSAVI analysis of this research can be seen in Table 29 (subplot results were not as good so are not fully discussed).

Table 29 Best performing predefined narrowband ROSAVI. Tests marked with asterisk are plotted below. Results are colour coded from blue (poor) to red (excellent).

Colour Scale (r^2_{cv})			ASD: Full Spectrum (705/750)				CHRIS M1: Spectral Subset (703/748)			
0 1			Subplot		Plot		Subplot		Plot	
Location	VZA	Variable	r^2_{cv}	RMSE _{cv}	r^2_{cv}	RMSE _{cv}	r^2_{cv}	RMSE _{cv}	r^2_{cv}	RMSE _{cv}
Herschel Island (2011)	0°	LCC*	0.08	6.43	0.77	3.38	0.13	6.33	0.77	3.40
		PAI _e	0.09	0.30	0.41	0.23	0.02	0.30	0.39	0.23
		CCC _e	0.17	0.12	0.55	0.08	0.09	0.12	0.54	0.08
Banks Island (2012)	0°	LCC	0.44	7.95	0.73	5.05	0.50	9.30	0.73	5.04
		PAI _e	0.57	0.19	0.73	0.10	0.53	0.18	0.74	0.10
		CCC _e	0.49	0.08	0.69	0.04	0.48	0.08	0.70	0.04
	-36°	LCC	0.47	8.24	0.74	5.93	0.47	8.80	0.75	5.91
		PAI _e	0.68	0.16	0.87	0.09	0.58	0.18	0.88	0.09
		CCC _e	0.53	0.08	0.92	0.04	0.54	0.08	0.92	0.04
	-55°	LCC	0.53	7.68	0.75	5.61	0.48	8.66	0.75	5.59
		PAI _e	0.67	0.16	0.90	0.10	0.54	0.19	0.90	0.10
		CCC _e	0.49	0.08	0.94	0.04	0.60	0.07	0.94	0.05
	+36°	LCC	0.30	10.15	0.74	5.72	0.29	9.77	0.74	5.73
		PAI _e	0.50	0.19	0.82	0.10	0.52	0.18	0.82	0.10
		CCC _e *	0.50	0.07	0.88	0.04	0.50	0.08	0.88	0.04
	+55°	LCC	0.47	8.25	0.69	6.13	0.52	8.45	0.69	6.11
		PAI _e	0.60	0.17	0.75	0.11	0.44	0.20	0.76	0.11
		CCC _e	0.44	0.08	0.81	0.05	0.52	0.08	0.81	0.05

<i>Richards Island (2013)</i>	0°	<i>LCC</i>	0.53	5.74	0.45	4.54	0.53	5.74	0.45	4.54
		<i>PAI_e</i>	0.51	0.20	0.57	0.25	0.51	0.20	0.57	0.25
		<i>CCC_e</i>	0.51	0.00	0.51	0.10	0.55	0.10	0.51	0.10
	-36°	<i>LCC</i>	0.61	5.94	0.51	4.24	0.60	5.93	0.50	4.25
		<i>PAI_e</i>	0.74	0.18	0.60	0.22	0.75	0.18	0.60	0.22
		<i>CCC_e</i>	0.73	0.10	0.53	0.08	0.74	0.10	0.54	0.08
	-55°	<i>LCC</i>	0.45	5.77	0.45	4.20	0.44	5.77	0.44	4.20
		<i>PAI_e</i>	0.73	0.19	0.53	0.21	0.73	0.18	0.53	0.21
		<i>CCC_e</i>	0.58	0.10	0.41	0.08	0.57	0.10	0.41	0.08
	+36°	<i>LCC</i>	0.51	5.61	0.40	4.45	0.50	5.61	0.39	4.44
		<i>PAI_e</i>	0.55	0.20	0.42	0.24	0.56	0.20	0.42	0.24
		<i>CCC_e</i>	0.46	0.10	0.46	0.10	0.46	0.10	0.46	0.10
	+55°	<i>LCC</i>	0.59	5.65	0.44	4.33	0.60	5.64	0.44	4.32
		<i>PAI_e*</i>	0.66	0.18	0.53	0.24	0.67	0.18	0.54	0.24
		<i>CCC_e</i>	0.73	0.10	0.51	0.10	0.74	0.09	0.53	0.10
<i>Richardson Mountains (2013)</i>	0°	<i>LCC</i>	0.40	5.64	0.44	4.82	0.39	5.72	0.42	4.89
		<i>PAI_e</i>	0.34	0.25	0.45	0.17	0.33	0.25	0.45	0.17
		<i>CCC_e</i>	0.18	0.11	0.41	0.09	0.17	0.11	0.40	0.09
	-36°	<i>LCC</i>	0.33	5.98	0.35	5.29	0.33	5.98	0.35	5.29
		<i>PAI_e</i>	0.25	0.26	0.35	0.20	0.24	0.26	0.22	0.19
		<i>CCC_e</i>	0.13	0.12	0.25	0.11	0.13	0.12	0.26	0.11
	-55°	<i>LCC</i>	0.53	6.22	0.52	5.31	0.52	6.21	0.53	5.31
		<i>PAI_e</i>	0.27	0.27	0.26	0.22	0.24	0.27	0.24	0.22
		<i>CCC_e</i>	0.29	0.12	0.39	0.11	0.27	0.12	0.39	0.11
	+36°	<i>LCC</i>	0.13	5.89	0.22	5.03	0.14	5.92	0.23	5.06
		<i>PAI_e</i>	0.31	0.24	0.49	0.17	0.31	0.24	0.49	0.17
		<i>CCC_e</i>	0.31	0.10	0.33	0.09	0.26	0.11	0.33	0.09
	+55°	<i>LCC</i>	0.34	6.01	0.52	5.23	0.35	6.03	0.53	5.26
		<i>PAI_e</i>	0.40	0.26	0.33	0.18	0.40	0.26	0.34	0.18
		<i>CCC_e</i>	0.18	0.11	0.32	0.10	0.18	0.11	0.32	0.10
<i>Richardson Mountains (2014)</i>	0°	<i>LCC</i>	0.02	3.84	0.48	2.08	0.08	3.91	0.52	2.04
		<i>PAI_e</i>	0.03	0.41	0.35	0.43	0.11	0.40	0.32	0.44
		<i>CCC_e</i>	0.04	0.17	0.39	0.18	0.01	0.18	0.37	0.18
	-36°	<i>LCC</i>	0.00	3.91	0.43	2.59	0.02	4.01	0.47	2.61
		<i>PAI_e</i>	0.01	0.41	0.49	0.53	0.05	0.41	0.51	0.52
		<i>CCC_e</i>	0.03	0.17	0.52	0.23	0.13	0.19	0.55	0.23
	-55°	<i>LCC</i>	0.00	4.15	0.56	2.45	0.14	3.93	0.56	2.42
		<i>PAI_e</i>	0.06	0.41	0.51	0.34	0.06	0.40	0.45	0.34
		<i>CCC_e</i>	0.19	0.16	0.56	0.14	0.05	0.17	0.56	0.14
	+36°	<i>LCC</i>	0.09	3.70	0.38	2.30	0.25	3.80	0.41	2.32
		<i>PAI_e</i>	0.09	0.40	0.50	0.42	0.25	0.38	0.51	0.42
		<i>CCC_e</i>	0.31	0.15	0.57	0.17	0.00	0.18	0.59	0.18
	+55°	<i>LCC</i>	0.01	3.82	0.33	2.17	0.14	3.82	0.35	2.15
		<i>PAI_e</i>	0.09	0.40	0.50	0.31	0.37	0.33	0.49	0.31
		<i>CCC_e</i>	0.30	0.14	0.54	0.13	0.00	0.18	0.53	0.13
<i>All Sites</i>	<i>Overall</i>		0.36	-	0.54	-	0.36	-	0.54	-
	<i>All</i>	<i>LCC</i>	0.33	6.03	0.52	4.33	0.35	6.16	0.52	4.33
	<i>All</i>	<i>PAI_e</i>	0.39	0.26	0.54	0.23	0.39	0.26	0.53	0.23
	<i>All</i>	<i>CCC_e</i>	0.36	0.11	0.55	0.10	0.33	0.12	0.55	0.10
	0°	<i>LCC</i>	0.29	5.92	0.57	3.97	0.33	6.20	0.58	3.98
	-36°	<i>LCC</i>	0.35	6.02	0.51	4.51	0.36	6.18	0.52	4.52
	-55°	<i>LCC</i>	0.38	5.96	0.57	4.39	0.40	6.14	0.57	4.38
	+36°	<i>LCC</i>	0.26	6.34	0.44	4.38	0.30	6.28	0.44	4.39

+55°	<i>LCC</i>	0.35	5.93	0.50	4.47	0.40	5.99	0.50	4.46
0°	<i>PAI_e</i>	0.31	0.27	0.50	0.24	0.30	0.27	0.49	0.24
-36°	<i>PAI_e</i>	0.42	0.25	0.58	0.26	0.41	0.26	0.55	0.26
-55°	<i>PAI_e</i>	0.43	0.26	0.55	0.22	0.39	0.26	0.53	0.22
+36°	<i>PAI_e</i>	0.36	0.26	0.56	0.23	0.41	0.25	0.56	0.23
+55°	<i>PAI_e</i>	0.44	0.25	0.53	0.21	0.47	0.24	0.53	0.21
0°	<i>CCC_e</i>	0.28	0.10	0.51	0.10	0.26	0.12	0.50	0.10
-36°	<i>CCC_e</i>	0.36	0.12	0.56	0.12	0.39	0.12	0.57	0.12
-55°	<i>CCC_e</i>	0.39	0.12	0.58	0.09	0.37	0.12	0.58	0.10
+36°	<i>CCC_e</i>	0.40	0.11	0.56	0.10	0.31	0.12	0.57	0.10
+55°	<i>CCC_e</i>	0.41	0.11	0.55	0.10	0.36	0.12	0.55	0.10
0°	<i>All</i>	0.29	-	0.53	-	0.30	-	0.53	-
-36°	<i>All</i>	0.38	-	0.55	-	0.38	-	0.55	-
-55°	<i>All</i>	0.40	-	0.57	-	0.39	-	0.56	-
+36°	<i>All</i>	0.34	-	0.52	-	0.34	-	0.52	-
+55°	<i>All</i>	0.40	-	0.52	-	0.41	-	0.53	-

The cross-validated ROSAVI regression analysis produced comparable mean r^2_{cv} values for all three vegetation variables, LCC ($r^2_{cv}=0.52$, $RMSE_{cv}=4.33$), PAI_e ($r^2_{cv}=0.54$, $RMSE_{cv}=1.10$), and CCC_e ($r^2_{cv}=0.55$, $RMSE_{cv}=0.10$) using the full spectrum dataset. Very similar results were produced with the M1 dataset: LCC ($r^2_{cv}=0.52$, $RMSE_{cv}=4.33$), PAI_e ($r^2_{cv}=0.53$, $RMSE_{cv}=0.23$), and CCC_e ($r^2_{cv}=0.55$, $RMSE_{cv}=0.10$), whereas the SR M1 results were markedly lower than the SR ASD results. The CCC_e variable showed the best correlation results with ROSAVI, as compared to PAI_e for the SR retrievals. Visualization of ROSAVI results can be seen in Figure 48. The performance of ROSAVI used with either the ASD or simulated M1 dataset did not vary noticeably across all testing variables (e.g. vegetation variables, VZAs, and field sites). For example, the VZA that produced the best mean results for all three vegetation variables was -55° ($r^2_{cv}=0.57$); however, r^2_{cv} values were all comparable, being within +/-0.04 for all VZAs. This suggests that extremely narrow pre-defined bands as those published for ROSAVI may not provide enhanced extraction capabilities as previously shown in the SR results. More likely, the ROSAVI wavelengths may not be optimal for the vegetation conditions of this study.

Figure 48 ROSAVI results across variables and datasets (upper left), variables and angles (upper right), angles and datasets for all variables combined (lower left), and sites and datasets for all variables combined (lower right). Boxplots are for the plot scale.

Similar field site-based results were found as for the SR analysis; e.g. Banks Island (2012) produced the highest correlations for all vegetation variables as compared to the other field sites (Figure 48). The r^2_{cv} values for Banks Island were high for all variables (e.g. for -55°: LCC, $r^2_{cv}=0.75$, $RMSE_{cv}=5.61$; PAI_e , $r^2_{cv}=0.90$, $RMSE_{cv}=0.10$; CCC_e , $r^2_{cv}=0.94$, $RMSE_{cv}=0.04$). All other field sites that were sampled with a multi-angle approach produced substantially poorer

results (Figure 48, bottom right). The Richardson Mountains (2013, 2014) and Richards Island (2013) field sites show comparable r^2_{cv} and $RMSE_{cv}$ ranges; however, it should be noted that the Herschel Island (2011) field campaign did not include multi-angle sampling, and therefore does not provide an adequate comparison. The strong results achieved for Banks Island may be due to the same reasons discussed with respect to the range of vegetation cover for SR in the previous section. Scatter plots showing predictions (measured vs. predicted) are shown below for various field sites with optimal predictive results (LCC, Herschel Island 0° ; PAI_e, Richards Island -55° ; CCC_e, Banks Island -36°) (Figure 49). All relationships demonstrate linear relationships, especially CCC_e for Banks Island. The scatter plots also demonstrate that almost identical relationships exist between the narrow bands of the ASD dataset and the slightly larger bandwidths of the M1 dataset, and suggest, contrary to what was found for the SR analysis, that a ~ 1 nm to ~ 10 nm difference does not provide significant improvement in results when bands are closely matched.

The VZA that produced the best mean correlations for all three vegetation variables (inclusive) was -55° (mean $r^2_{cv}=0.57$ and $r^2_{cv}=0.56$) for the full ASD dataset and M1 dataset, respectfully; however, mean r^2_{cv} values for each angle was comparable.

Figure 49 Various results for the ROSAVI modelling. Results for ASD narrow bands (left column) closely match the results for the resampled larger M1 bandwidth. Scatter plots are for the plot scale.

5.3.3. Non-parametric multi-variate regression: Gaussian Processes Regression (GPR)

5.3.3.1. GPR modelling results

The results for GPR modelling are shown in Table 30 for both the ASD and M1 datasets for all vegetation variables and measurement scenarios using a similar colour gradient to previous analyses. These results show that including all narrow spectral bands in the GPR model did not lead to the best performance ($r^2_{cv}=0.56$), as compared to using a spectral subset (i.e. the simulated CHRIS/PROBA M1 dataset) ($r^2_{cv}=0.62$), and this confers with a previous study by (Verrelst et al., 2016). As for parametric regression, sampling at the plot scale is better as spectra measured at the subplot scale for both datasets generally produced inferior results (ASD, subplot mean $r^2_{cv}=0.41$; M1 subplot mean $r^2_{cv}=0.48$). Only the Richards Island (2013) and Richardson Mountains (2013) sites produced comparable results at the subplot and plot scales.

Table 30 GPR results showing the overall best r^2_{cv} model and associated $RMSE_{cv}$ values for the field-scale analysis using the ASD full spectrum and M1 spectral subset for both subplot and plot spatial scales. GPR-100: 100 bands were removed in each iteration. GPR-1: One band was removed in each iteration. Plotted relationships are bolded and marked with an asterisk.

Colour Scale (r^2_{cv})			ASD (GPR-100): Full Spectrum				CHRIS M1 (GPR-1): Spectral Subset			
0 1			Subplot		Plot		Subplot		Plot	
Location	Angle	Variable	r^2_{cv}	$RMSE_{cv}$	r^2_{cv}	$RMSE_{cv}$	r^2_{cv}	$RMSE_{cv}$	r^2_{cv}	$RMSE_{cv}$
Herschel Island (2011)	0°	LCC*	0.14	6.12	0.47	4.52	0.17	5.72	0.77	3.43
		PAI _e	0.22	0.29	0.27	0.25	0.25	0.24	0.37	0.26
		CCC _e	0.30	0.11	0.43	0.08	0.28	0.10	0.45	0.08
Banks Island (2012)	0°	LCC	0.67	6.46	0.77	3.82	0.53	6.82	0.78	3.77
		PAI _e	0.58	0.18	0.84	0.10	0.51	0.18	0.78	0.10
		CCC _e	0.55	0.08	0.85	0.04	0.55	0.07	0.79	0.04
	-36°	LCC	0.63	6.98	0.74	4.89	0.67	6.92	0.78	4.32
		PAI _e	0.68	0.15	0.69	0.16	0.67	0.15	0.93	0.08
		CCC _e *	0.52	0.07	0.91	0.04	0.59	0.06	0.92	0.04
	-55°	LCC	0.68	6.48	0.72	7.97	0.70	6.59	0.70	5.14
		PAI _e *	0.64	0.16	0.96	0.10	0.65	0.16	0.96	0.10
		CCC _e	0.52	0.07	0.94	0.05	0.53	0.07	0.92	0.05
	+36°	LCC	0.58	7.49	0.69	7.50	0.47	8.65	0.75	6.31
		PAI _e	0.56	0.17	0.83	0.12	0.68	0.15	0.87	0.12
		CCC _e	0.42	0.07	0.88	0.05	0.59	0.06	0.88	0.05
	+55°	LCC	0.57	7.53	0.75	6.56	0.58	7.77	0.80	5.55
		PAI _e	0.64	0.16	0.72	0.17	0.63	0.16	0.88	0.11
		CCC _e	0.46	0.07	0.71	0.07	0.57	0.06	0.88	0.05
Richards Island (2013)	0°	LCC	0.45	4.98	0.69	4.39	0.62	4.98	0.68	3.97
		PAI _e	0.95	0.20	0.66	0.21	0.78	0.20	0.76	0.18
		CCC _e	0.66	0.10	0.67	0.10	0.75	0.10	0.84	0.09
	-36°	LCC	0.52	5.02	0.74	3.97	0.50	4.98	0.63	3.97
		PAI _e	0.82	0.20	0.54	0.22	0.70	0.17	0.64	0.19
		CCC _e	0.75	0.10	0.70	0.11	0.61	0.08	0.61	0.08
	-55°	LCC	0.58	4.98	0.64	3.97	0.67	4.98	0.79	3.97
		PAI _e	0.52	0.22	0.61	0.23	0.74	0.21	0.73	0.21
		CCC _e	0.50	0.10	0.66	0.11	0.47	0.09	0.78	0.11
	+36°	LCC	0.64	4.98	0.66	4.52	0.78	4.98	0.71	3.97
		PAI _e	0.58	0.20	0.58	0.24	0.88	0.18	0.68	0.18
		CCC _e	0.35	0.10	0.71	0.10	0.91	0.10	0.67	0.10
	+55°	LCC	0.33	5.15	0.63	3.98	0.66	4.98	0.67	3.97
		PAI _e	0.95	0.20	0.52	0.21	0.81	0.19	0.52	0.18
		CCC _e	0.64	0.10	0.84	0.10	0.63	0.10	0.44	0.11
Richardson Mountains (2013)	0°	LCC	0.26	5.96	0.25	4.82	0.36	5.54	0.56	4.49
		PAI _e	0.35	0.26	0.30	0.22	0.47	0.25	0.46	0.19
		CCC _e	0.26	0.12	0.35	0.10	0.51	0.11	0.51	0.08
	-36°	LCC	0.31	5.97	0.29	5.15	0.33	5.34	0.47	5.05
		PAI _e	0.30	0.26	0.31	0.22	0.57	0.26	0.42	0.21
		CCC _e	0.35	0.11	0.31	0.11	0.44	0.12	0.67	0.11
	-55°	LCC	0.60	5.72	0.36	4.98	0.85	5.60	0.42	5.04
		PAI _e	0.45	0.26	0.35	0.22	0.73	0.26	0.61	0.22
		CCC _e	0.43	0.12	0.48	0.11	0.73	0.12	0.54	0.11
	+36°	LCC	0.36	5.73	0.43	5.01	0.44	5.59	0.37	4.94
		PAI _e	0.22	0.26	0.28	0.22	0.34	0.26	0.56	0.19
		CCC _e	0.30	0.12	0.41	0.11	0.38	0.11	0.57	0.10

Richardson Mountains (2014)	+55°	LCC	0.36	5.72	0.46	4.93	0.32	5.72	0.30	5.05
		PAI _e	0.18	0.26	0.21	0.22	0.45	0.26	0.30	0.21
		CCC _e	0.47	0.12	0.44	0.11	0.38	0.12	0.57	0.11
	0°	LCC	0.06	3.74	0.48	2.20	0.13	3.83	0.51	2.40
		PAI _e	0.06	0.39	0.51	0.44	0.06	0.42	0.53	0.41
		CCC _e	0.14	0.20	0.39	0.18	0.10	0.16	0.34	0.18
	-36°	LCC	0.02	3.16	0.67	2.15	0.15	3.73	0.40	1.82
		PAI _e	0.22	0.38	0.50	0.43	0.14	0.39	0.57	0.43
		CCC _e	0.06	0.15	0.51	0.18	0.09	0.17	0.55	0.18
	-55°	LCC	0.15	3.02	0.65	2.30	0.11	3.83	0.56	2.31
		PAI _e	0.12	0.41	0.46	0.41	0.43	0.38	0.62	0.43
		CCC _e	0.16	0.13	0.40	0.18	0.38	0.15	0.56	0.18
	+36°	LCC	0.16	3.10	0.43	2.21	0.03	4.22	0.42	2.32
		PAI _e	0.04	0.44	0.22	0.40	0.20	0.38	0.47	0.37
		CCC _e	0.22	0.13	0.29	0.18	0.12	0.16	0.54	0.16
	+55°	LCC	0.06	3.18	0.58	2.12	0.26	4.30	0.55	2.10
		PAI _e	0.10	0.41	0.32	0.40	0.18	0.39	0.47	0.39
		CCC _e	0.15	0.15	0.42	0.18	0.22	0.15	0.55	0.17
All sites	Overall	0.41	-	0.56	-	0.48	-	0.62	-	
All	All	LCC	0.39	5.31	0.58	4.38	0.44	5.48	0.60	3.99
	All	PAI _e	0.44	0.26	0.51	0.25	0.52	0.25	0.63	0.23
	All	CCC _e	0.39	0.11	0.59	0.11	0.47	0.11	0.65	0.10
	0°	LCC	0.32	5.45	0.53	3.95	0.36	5.38	0.66	3.61
	-36°	LCC	0.37	5.28	0.61	4.04	0.41	5.24	0.57	3.79
	-55°	LCC	0.50	5.05	0.59	4.81	0.58	5.25	0.62	4.12
	+36°	LCC	0.44	5.33	0.55	4.81	0.43	5.86	0.56	4.39
	+55°	LCC	0.33	5.40	0.61	4.40	0.46	5.69	0.58	4.17
	0°	PAI _e	0.43	0.26	0.52	0.24	0.41	0.26	0.58	0.23
	-36°	PAI _e	0.51	0.25	0.51	0.26	0.52	0.24	0.64	0.23
	-55°	PAI _e	0.43	0.26	0.60	0.24	0.64	0.25	0.73	0.24
	+36°	PAI _e	0.35	0.27	0.48	0.25	0.53	0.24	0.65	0.22
	+55°	PAI _e	0.47	0.26	0.44	0.25	0.52	0.25	0.54	0.22
	0°	CCC _e	0.38	0.12	0.54	0.10	0.44	0.11	0.59	0.10
	-36°	CCC _e	0.42	0.11	0.61	0.11	0.43	0.11	0.69	0.10
	-55°	CCC _e	0.40	0.10	0.62	0.11	0.53	0.11	0.70	0.11
	+36°	CCC _e	0.32	0.10	0.57	0.11	0.50	0.11	0.67	0.10
	+55°	CCC _e	0.43	0.11	0.60	0.11	0.45	0.11	0.61	0.11
	0°	All	0.38	-	0.53	-	0.40	-	0.61	-
	-36°	All	0.43	-	0.58	-	0.46	-	0.63	-
	-55°	All	0.45	-	0.60	-	0.58	-	0.68	-
	+36°	All	0.37	-	0.53	-	0.49	-	0.62	-
	+55°	All	0.41	-	0.55	-	0.47	-	0.58	-

An examination of the cross-validated r^2_{cv} values for sequentially removed, least contributing bands for each of the GPR models shows that results remain stable as bands are removed from models, and this is similar across all VZAs and vegetation variables (i.e. LCC, PAI_e, and CCC_e). For example, the ASD dataset does not show substantial improvement for all variables as bands

are eliminated (Figure 50). Some slight overall gains/trends are visible for PAI_e and CCC_e at all VZAs (i.e. VZA tests all follow the same pattern), but not LCC where a wider variation is seen in the results as bands are removed. The average cross-validated r^2_{cv} of LCC across VZAs shows almost no gains as more bands are removed.

Figure 50 Coefficient of determination (r^2_{cv}) values for the full spectrum ASD dataset for all variables and all angles. Field sites have been combined into one value. Plot scale results are shown.

As expected, the associated cross-validated $RMSE_{cv}$ values for all vegetation variables show an overall (although slight) decrease as bands are eliminated from the models (Figure 51), particularly when there are fewer than about 130 bands. The exception is PAI_e at 0° , where the overall $RMSE_{cv}$ increases when there are fewer than about 225 bands and bands are further removed from the model, even when its associated r^2_{cv} values increase.

Figure 51 $RMSE_{cv}$ values for the ASD spectral dataset. All field sites have been combined into one value. Values are for the plot scale.

The cross-validated r^2_{cv} values for the M1 spectral subset show very similar overall prediction trends to the full spectrum dataset. Figure 52 shows the sequentially removed, least contributing bands for each of the GPR models for LCC, PAI_e , and CCC_e across all VZAs. As reported previously, the spectral subset performed better than the full spectrum dataset; however, the results shown here remain stable until relatively few bands remained. For LCC, results were stable until approximately 10 bands were left, whereas for PAI_e and CCC_e , results were stable until there were as few as 4 bands left. For all variables, using only one or two bands produced the worst overall results, indicating that optimal models would require 5-10 bands for satisfactory/optimal performance.

Figure 52 ASD-M1 coefficient of determination (r^2_{cv}) values for the various vegetation variables and look angles. All field sites have been combined. Values are for the plot scale.

The associated $RMSE_{cv}$ values for all vegetation variables processed with the spectral subset are relatively stable as bands are removed, except for PAI_e which shows an overall diminishing trend (i.e. better $RMSE_{cv}$ values). LCC and CCC_e show slight overall decreases; however, CCC_e becomes rather unstable when fewer than 10 bands remain. $RMSE_{cv}$ values are shown in Figure 53. It can be seen that for PAI_e and CCC_e $RMSE_{cv}$ jumps up when ~ 2 bands remain. Such phenomena are likely attributable to variables being kicked out of the model that serve better as combination-predictors than the remaining bands do as individual/singular predictors.

Figure 53 M1 dataset $RMSE_{cv}$ for LCC, PAI_e , and CCC_e . All field sites have been combined. Values are for plot scale.

The cross-validated GPR analysis produced overall higher mean r^2_{cv} (correlation) values for CCC_e ($r^2_{cv}=0.65$, $RMSE_{cv}=0.10$) than for LCC ($r^2_{cv}=0.60$, $RMSE_{cv}=3.99$) or PAI_e ($r^2_{cv}=0.63$, $RMSE_{cv}=0.23$) using the simulated CHRIS/PROBA M1 spectral subset. Visualization of these results can be seen in Figure 54; however, GPR retrievals of all vegetation variables are quite similar (e.g. median values). What is particularly evident in Figure 54 is that in every case, the M1 spectral subset outperformed the full ASD spectral dataset.

A breakdown of the results with respect to VZA is shown in Figure 54 (bottom right). The -55° VZA produced the best overall results (e.g. $r^2_{cv}=0.68$, mean of M1 datasets), while the worst were 0° (e.g. $r^2_{cv}=0.61$, mean of M1 datasets) and $+55^\circ$ (e.g. $r^2_{cv}=0.58$, mean of M1 datasets).

Figure 54 GPR results for all field sites, angles, and variables. Values are for plot scale measurements.

Similar regionally based results are reported here as compared to the SR and ROSAVI analysis; Banks Island (2012) produced the best correlation results for all vegetation variables (Figure 54). The r^2_{cv} values were high for all variables (e.g. for -55°: LCC, $r^2_{cv}=0.70$, $RMSE_{cv}=5.14$; PAI_e , $r^2_{cv}=0.96$, $RMSE_{cv}=0.10$; CCC_e , $r^2_{cv}=0.92$, $RMSE_{cv}=0.05$). The Richardson Island (2013) field site showed the second highest r^2_{cv} and lowest $RMSE_{cv}$ values, unlike the previous parametric regression results. As for SR and ROSAVI, the strong results achieved for Banks Island may be due to the large spatial variation in vegetation PAI_e values and the way in which sites were sampled, as previously suggested for the SR and ROSAVI analysis. Scatter plots showing selected best predictions/correlations (measured vs. predicted) are given in Figure 55 for various field sites (LCC, Herschel Island 0°; PAI_e , Banks Island -55°; CCC_e ; Banks Island -36°). All demonstrate linear relationships, especially the PAI_e and CCC_e plots for Banks Island.

Figure 55 GPR predictions for the vegetation variables at various view zenith angles.

5.3.3.2. Gaussian Processes Regression: Spectral band analysis

The GPR band analysis tool (BAT) ranked the bands, outputting the frequency of the top band used in 10-fold cross-validated regressions and which band had the highest contribution to the final best model (i.e. the best single variable). Hyperparameter values (l_b), on which the band rankings are based, are discussed first. The results are presented for both the full spectrum ASD dataset and simulated CHRIS/PROBA M1 dataset at the plot level.

The l_b values for the cross-validated GPR models for LCC, PAI_e, and CCC_e processed from the full-spectrum ASD dataset can be seen in Figure 56. Large differences in the l_b values are evident for all variables and at all VZAs. It is important to note that there are very few spectral regions with informative wavelengths/bands (low l_b values), but many regions with particularly poorly informative bands (high l_b values); furthermore, there exists large differences in l_b values between VZAs for each vegetation variable. For example, LCC at -55° and $+55^\circ$ show low l_b values for the RE at approximately 720 nm, but for the remaining VZAs, sigma values rise to very high values suggesting that these bands around 720 nm, at these view angles, can be problematic in the regression algorithm (Figure 56, top right). However, since the GPR is a data-driven algorithm, and the l_b values depend upon the data used in the training phase, l_b values may fluctuate depending on the given training-validation partitioning (Verrelst et al., 2016). What is particularly surprising l_b for all vegetation variables is the large difference in l_b between view zenith angles and within the respective spectrally meaningful regions related to chlorophyll absorption and structurally-based (leaf and canopy) reflectance (Figure 56).

Figure 56 ASD l_b values for each vegetation variable and look angle. All field sites have been combined into one measurement. Values are for plot scale measurements.

The CHRIS/PROBA M1 dataset l_b values showed overall less volatility than for the full ASD dataset (Figure 57). However, once again there appeared to be significant differences in l_b values for the different VZAs for the same vegetation variable – and values that don't make physical sense for the variable in question. For example, LCC values show overall poor band performance in the red-edge regions for all VZAs.

Figure 57 M1 l_b values for the various field variables and look angles. All field sites have been combined into one measurement. Values are for the plot scale analysis.

Table 31 shows the best contributing (best predictive power) and top-ranking (most used across model iterations) cross-validated bands for all vegetation variables, VZAs, and spatial and spectral subsets. The weighted mean for each variable's optimal spectral bands was calculated using the associated r^2_{cv} values to determine a more meaningful spectral centre. Overall, it was shown that LCC benefitted from meaningful bands in the pigment absorption (VIS) and RE spectral regions

(593-731 nm). PAI_e benefitted from meaningful bands in the same spectral regions (609-757 nm), and CCC_e also benefitted most from spectral bands in the chlorophyll absorption region and red-edge (598-721 nm). Histograms of the simulated M1 dataset GPR band selections from Table 31 can be seen in Figures 58 and 59.

Table 31 Best bands (highest predictive power) and highest ranked bands (most common band selected across all GPR models) from GPR-BAT analysis for the M1 spectral subset. It is not known if band differences are due to spatial scale or some other factor.

			<i>ASD (GPR-100) Full Spectrum</i>				<i>CHRIS M1 (GPR-1) Spectral Subset</i>			
			<i>Subplot</i>		<i>Plot</i>		<i>Subplot</i>		<i>Plot</i>	
<i>Location</i>	<i>Angle</i>	<i>Variable</i>	<i>Best</i>	<i>Rank</i>	<i>Best</i>	<i>Rank</i>	<i>Best</i>	<i>Rank</i>	<i>Best</i>	<i>Rank</i>
<i>Herschel Island (2011)</i>	0°	<i>LCC</i>	777	1040	800	738	680	680	442	590
		<i>PAI_e</i>	603	338	850	540	680	672	461	672
		<i>CCC_e</i>	680	349	641	345	442	551	461	672
<i>Banks Island (2012)</i>	0°	<i>LCC</i>	985	1053	740	724	997	411	411	709
		<i>PAI_e</i>	439	412	456	405	411	411	680	590
		<i>CCC_e</i>	739	337	786	502	411	442	680	683
	-36°	<i>LCC</i>	950	383	477	507	940	925	411	471
		<i>PAI_e</i>	884	1063	995	700	709	411	411	461
		<i>CCC_e</i>	402	427	894	533	461	411	748	530
	-55°	<i>LCC</i>	400	1063	827	710	411	411	411	719
		<i>PAI_e</i>	1022	441	677	695	411	411	680	680
		<i>CCC_e</i>	750	699	661	535	703	411	680	606
	$+36^\circ$	<i>LCC</i>	987	395	859	730	411	411	411	510
		<i>PAI_e</i>	852	671	936	887	411	411	940	680
		<i>CCC_e</i>	881	1002	680	711	411	411	940	680
	$+55^\circ$	<i>LCC</i>	940	728	546	712	411	411	411	546
		<i>PAI_e</i>	959	405	579	559	411	411	411	940
		<i>CCC_e</i>	401	419	553	567	680	442	748	683
<i>Richards Island (2013)</i>	0°	<i>LCC</i>	823	775	768	775	411	676	940	925
		<i>PAI_e</i>	789	769	817	344	777	583	680	735
		<i>CCC_e</i>	783	775	837	395	680	748	755	510
	-36°	<i>LCC</i>	365	822	675	695	742	703	755	728
		<i>PAI_e</i>	676	703	775	957	748	708	895	698
		<i>CCC_e</i>	660	822	681	957	748	735	808	683
	-55°	<i>LCC</i>	537	536	540	551	703	619	686	540
		<i>PAI_e</i>	973	623	664	600	762	722	940	682
		<i>CCC_e</i>	575	623	673	528	762	629	680	672
	$+36^\circ$	<i>LCC</i>	516	682	509	518	680	600	680	442
		<i>PAI_e</i>	453	674	604	1024	915	540	915	642
		<i>CCC_e</i>	474	676	515	677	940	505	703	610
	$+55^\circ$	<i>LCC</i>	465	468	463	479	661	457	833	452
		<i>PAI_e</i>	462	479	1003	522	691	697	940	940
		<i>CCC_e</i>	468	479	532	462	691	691	940	811
<i>Richardson Mountains (2013)</i>	0°	<i>LCC</i>	1009	1050	643	683	651	694	651	621
		<i>PAI_e</i>	780	681	779	680	590	777	808	912
		<i>CCC_e</i>	530	751	598	707	603	742	572	722
	-36°	<i>LCC</i>	604	799	768	751	703	716	709	807

		PAI_e	716	706	462	710	452	691	452	452
		CCC_e	561	702	533	709	540	635	703	709
	-55°	LCC	745	747	752	747	987	748	680	745
		PAI_e	913	949	941	1037	461	915	452	940
		CCC_e	976	728	1027	949	976	976	672	844
	$+36^\circ$	LCC	717	823	910	821	886	807	895	709
		PAI_e	914	717	726	710	940	680	940	716
		CCC_e	710	470	490	717	461	471	940	686
	$+55^\circ$	LCC	1042	715	842	1059	755	713	748	697
		PAI_e	986	711	941	1001	940	551	940	696
		CCC_e	1039	1010	943	1010	905	709	452	709
<i>Richardson Mountains (2014)</i>	0°	LCC	924	364	738	388	622	411	777	686
		PAI_e	728	721	778	378	709	703	925	770
		CCC_e	742	352	741	378	770	411	925	691
	-36°	LCC	486	926	537	556	940	461	471	742
		PAI_e	931	930	1004	556	709	709	481	672
		CCC_e	767	1062	1023	556	703	703	622	621
	-55°	LCC	678	1060	792	765	603	572	703	709
		PAI_e	729	711	529	981	442	955	691	621
		CCC_e	628	703	904	718	442	965	641	551
	$+36^\circ$	LCC	555	379	721	725	461	886	735	722
		PAI_e	703	551	716	375	755	709	762	745
		CCC_e	862	456	404	389	703	709	762	600
	$+55^\circ$	LCC	400	344	733	713	490	411	716	713
		PAI_e	599	381	1015	633	520	691	709	703
		CCC_e	659	527	1020	633	471	641	709	955
<i>All sites</i>		<i>Overall</i>	720	673	720	650	661	614	686	672
	<i>All</i>	LCC	727	731	686	674	688	606	620	640
	<i>All</i>	PAI_e	757	652	759	670	636	617	711	707
	<i>All</i>	CCC_e	673	639	721	610	663	617	723	666
	0°	LCC	922	946	748	675	671	583	625	707
	-36°	LCC	666	632	588	606	833	774	578	659
	-55°	LCC	563	816	729	688	714	601	611	664
	$+36^\circ$	LCC	718	588	738	683	655	606	636	561
	$+55^\circ$	LCC	825	642	625	718	573	481	649	578
	0°	PAI_e	673	614	691	430	631	599	717	722
	-36°	PAI_e	780	849	858	734	652	608	554	566
	-55°	PAI_e	959	647	684	776	532	737	700	722
	$+36^\circ$	PAI_e	692	676	779	844	741	537	901	690
	$+55^\circ$	PAI_e	690	471	825	614	645	578	675	855
	0°	CCC_e	717	548	745	459	568	629	677	639
	-36°	CCC_e	563	683	814	682	595	597	725	626
	-55°	CCC_e	744	684	774	643	764	755	671	659
	$+36^\circ$	CCC_e	728	697	560	661	679	483	844	647
	$+55^\circ$	CCC_e	623	612	698	623	706	610	705	773
	0°	<i>All</i>	757	684	728	522	620	605	671	690
	-36°	<i>All</i>	677	733	747	671	688	655	623	615
	-55°	<i>All</i>	745	721	730	701	663	697	663	683
	$+36^\circ$	<i>All</i>	713	647	686	723	694	539	801	636
	$+55^\circ$	<i>All</i>	703	566	706	655	641	557	677	734

Figure 58 Best overall band selections for each vegetation variable and VZA. Field sites have been combined into one value. Values are for plot scale measurements.

Figure 59 Highest overall ranking bands for each vegetation variable and VZA. Field sites have been combined into one value. Values are for plot scale measurements.

An interesting result is the selection of sensitive bands at the far ends of the spectrum (e.g. 400 nm and 900 nm, as seen in Table 31), and the fact that all vegetation variables elicit similar spectral responses (similar bands being chosen; see Figures 58 and 59). This can be explained by mechanisms of variable covariation (Olliger, 2011). Measured leaf and canopy variables of the same target are interrelated (Olliger, 2011, Verrelst et al., 2016). Given that both biochemical, biophysical, and soil properties govern the top-of-canopy reflectance, covariation relationships can play an important role in understanding spectral responses (Ollinger, 2011). This is demonstrated for LCC, PAI_e, and CCC_e (which is a derivative of the former variables). Important band selections for all variables show consistency within the ~450-500 nm (adjacent to peak green reflectance ~550 nm) and ~650-750 nm (chlorophyll absorption and red-edge) ranges. It is also visible in Figures 58 and 59 that band selection regions for all variables show consistency across the VZAs for the same spectral regions (~400-500 nm and ~650-750 nm).

Finally, the weighted bands were graphed in relation to VZA (Figure 60). The weighted best band selections using the M1 dataset showed no distinct spectral shift in relation to VZA as reported for the SR band selections. However, band selections using the GPR analysis appeared to produce a much higher degree of variation as compared to SR band selections (Figure 45). In some instances, band selections appear to follow the reflectance distribution as it relates to the intensity of reflectance across each of the VZAs (i.e. greatest reflectance in the negative view angles and least at nadir); however, this result is not consistent with the SR optimal band findings.

Figure 60 GPR band selections for each vegetation variable in relation to VZA. Averaged values show no increase in wavelength as look angles progress into forward scatter reflectance.

5.3.4. Summary of prediction results (*SR*, *ROSAVI*, and *GPR*)

All plot scale results based on the NRMSE_{cv} are presented in Table 32 below. NRMSE_{cv} values are presented using a red/white/blue colour ramp to highlight poor (blue, $\text{NRMSE}_{\text{cv}}=0.30$) to median (white, $\text{NRMSE}_{\text{cv}}=0.15$) to optimal results (red, $\text{NRMSE}_{\text{cv}}=0.0$). When all vegetation variables (LCC , PAI_e , and CCC_e) and VZAs were averaged across field sites, it was shown that

the SR produced the best model accuracies ($\text{NRMSE}_{\text{cv}}=0.12$, for the ASD full spectrum dataset) as compared to ROSAVI ($\text{NRMSE}_{\text{cv}}=0.16$, for the ASD full spectrum dataset) and GPR ($\text{NRMSE}_{\text{cv}}=0.16$, for the CHRIS M1 dataset). These results contrast with the r^2_{cv} results, where GPR produced the top correlations ($r^2_{\text{cv}}=0.62$), followed by SR ($r^2_{\text{cv}}=0.58$) then ROSAVI ($r^2_{\text{cv}}=0.54$) for the same datasets.

Table 32 NRMSE_{cv} results for SR, ROSAVI, and GPR. Results calculated across field sites have been combined.

<i>Colour Scale (NRMSE_{cv})</i>			<i>ASD: Full Spectrum</i>			<i>CHRIS M1: Spectral Subset</i>			<i>All</i>
			<i>SR</i>	<i>ROSAVI</i>	<i>GPR</i>	<i>SR</i>	<i>ROSAVI</i>	<i>GPR</i>	<i>All</i>
<i>Location</i>	<i>Angle</i>	<i>Variable</i>	<i>NRMSE_{cv}</i>	<i>NRMSE_{cv}</i>	<i>NRMSE_{cv}</i>	<i>NRMSE_{cv}</i>	<i>NRMSE_{cv}</i>	<i>NRMSE_{cv}</i>	<i>NRMSE_{cv}</i>
<i>All</i>	<i>All</i>	<i>LCC</i>	0.11	0.14	0.14	0.11	0.14	0.13	0.13
	<i>All</i>	<i>PAI_e</i>	0.15	0.20	0.22	0.17	0.20	0.20	0.19
	<i>All</i>	<i>CCC_e</i>	0.11	0.14	0.15	0.12	0.14	0.14	0.13
	<i>0°</i>	<i>LCC</i>	0.10	0.12	0.12	0.10	0.12	0.11	0.11
	<i>-36°</i>	<i>LCC</i>	0.11	0.14	0.13	0.12	0.14	0.12	0.13
	<i>-55°</i>	<i>LCC</i>	0.11	0.14	0.15	0.11	0.14	0.13	0.13
	<i>+36°</i>	<i>LCC</i>	0.11	0.14	0.15	0.11	0.14	0.14	0.13
	<i>+55°</i>	<i>LCC</i>	0.11	0.14	0.14	0.11	0.14	0.13	0.13
	<i>0°</i>	<i>PAI_e</i>	0.14	0.21	0.22	0.17	0.22	0.21	0.20
	<i>-36°</i>	<i>PAI_e</i>	0.15	0.22	0.23	0.16	0.21	0.20	0.20
	<i>-55°</i>	<i>PAI_e</i>	0.15	0.19	0.21	0.17	0.19	0.21	0.19
	<i>+36°</i>	<i>PAI_e</i>	0.16	0.20	0.21	0.17	0.20	0.19	0.19
	<i>+55°</i>	<i>PAI_e</i>	0.15	0.19	0.22	0.16	0.19	0.19	0.18
	<i>0°</i>	<i>CCC_e</i>	0.10	0.13	0.14	0.11	0.13	0.13	0.12
	<i>-36°</i>	<i>CCC_e</i>	0.12	0.16	0.15	0.13	0.16	0.14	0.14
	<i>-55°</i>	<i>CCC_e</i>	0.12	0.13	0.16	0.12	0.13	0.16	0.14
	<i>+36°</i>	<i>CCC_e</i>	0.11	0.14	0.15	0.12	0.14	0.14	0.13
	<i>+55°</i>	<i>CCC_e</i>	0.11	0.13	0.16	0.12	0.13	0.15	0.13
	<i>0°</i>	<i>All</i>	0.12	0.16	0.16	0.12	0.16	0.15	0.15
	<i>-36°</i>	<i>All</i>	0.13	0.18	0.17	0.14	0.17	0.15	0.16
	<i>-55°</i>	<i>All</i>	0.13	0.15	0.17	0.14	0.16	0.17	0.15
	<i>+36°</i>	<i>All</i>	0.13	0.16	0.17	0.13	0.16	0.16	0.15
	<i>+55°</i>	<i>All</i>	0.12	0.15	0.17	0.13	0.15	0.16	0.15
<i>All</i>	<i>All</i>	<i>All</i>	0.12	0.16	0.17	0.13	0.16	0.16	-

The vegetation variables that were best predicted across all sites were LCC (mean value across all VZAs and datasets; $\text{NRMSE}_{\text{cv}}=0.13$) and CCC_e ($\text{NRMSE}_{\text{cv}}=0.13$), followed by PAI_e ($\text{NRMSE}_{\text{cv}}=0.19$). Once again, mean prediction (i.e. accuracy) results contrast with the r^2_{cv} results, where PAI_e produced the best overall results (mean $r^2_{\text{cv}}=0.61$ at the plot scale) as compared to

CCC_e and LCC (mean $r^2_{cv}=0.55$ and $r^2_{cv}=0.51$, respectively). However, all results (i.e. accuracies and model correlations) were not considered to be markedly different; such comparable results may reflect the spectral similarities between variables (as previously discussed). Finally, combined mean prediction results showed that all VZAs produced similar NRMSE_{cv} (e.g. mean values for all combined datasets NRMSE_{cv}=0.15±0.01); however, r^2_{cv} results showed that -55° VZA was the best, albeit not markedly different than the other VZAs.

5.4. Discussion and Conclusion

A ground-based, multi-angle, multi-method spectroscopic analysis of Arctic vegetation was conducted across a bioclimatic gradient in the Western Canadian Arctic between the years 2011 to 2014. Key findings of these assessments are presented here with respect to the following: (1) the multi-angle spectral characterization of Arctic tundra; (2) the performance of a multi-band narrowband vegetation index (VI) across various spatial, spectral, and angular domains and the assessment of the optimal band selections relating to vegetation variables and view zenith angles; (3) the performance of predefined narrowband vegetation indices across various spatial, spectral, and angular domains; (4) the performance of Gaussian Processes Regression across various spatial, spectral, and angular domains and the assessment of optimal band selections relating to vegetation variables and view zenith angles; and (5) the overall conclusions that were applied the empirical studies of Chapters 6 and 7 .

(1) The multi-angle spectroscopic analysis of Arctic tundra vegetation across all field sites showed that top-of-canopy reflectance possessed angular dependencies and that the greatest variability in the reflectance signals appeared in the VIS/RE regions, specifically in all regions below ~500 nm and in regions between ~600-700 nm (with peak variability at ~680 nm, i.e. chlorophyll absorption). All regions showed the least degree of spectral variability at ~550 nm (i.e.

peak green reflectance) and in longer wavelengths from the RE into the NIR (~700 nm and above) (i.e. reflectance related to leaf and canopy structure). The low reflectance variability observed at all sites around ~550 nm may be due to consistent quantities of leaf/canopy carotenoid content (i.e. xanthophylls) found within and across Arctic vegetation species/assemblages. Previous studies have shown that carotenoids affect the reflectance spectrum between ~500 nm to 550 nm, with changing sensitivity according to species (Fillela et al., 1996; Gamon et al., 1990; Gamon et al., 1993; Zarco-Tejada et al., 2000; Stagakis et al., 2014). The high variability of reflectance found at ~680 nm may be attributable to a high degree of leaf/canopy chlorophyll differences found between species/sites, especially as it relates to the timing of measurements (i.e. weather variability, seasonality). Since chlorophyll degrades rapidly in comparison to carotenoids when plants undergo stress or senescence (Merzlyak & Gitelson, 1995; Sims & Gamon, 2002; Croft et al., 2013), the large differences in variability between these two spectral regions (i.e. chlorophyll:carotenoid ratios) may point towards an enhanced means of better understanding seasonal changes across a variety of environmental conditions, species, and functional types that are found in the Arctic (Stagakis et al., 2014; Garbulsky et al., 2011). The field spectra showed no observable patterns related to variability across the various VZAs.

It was found that negative VZAs produced the greatest overall reflectance values compared to nadir and positive VZAs. This is as expected for hot-spot backscatter spectra where shadows are minimized by the relatively small angular difference between the sensor and illumination source (i.e. the sun), while forward scattering observations contain more signal from shaded leaves and branches. Interestingly, nadir spectral measurements produced the overall smallest reflectance values across all spectral ranges (in each spectral region - VI, RE, NIR), providing evidence that tundra does not act as a specular or diffuse reflector (more related to volume scattering) and that,

like other ecosystems, nadir measurements are highly affected by canopy gaps and shadows (due to hummocks) (Stagakis et al., 2010). Increased canopy gap fraction has been said to decrease the quality and often the magnitude of the reflectance signal (Deering et al., 1999; Sandmeier et al., 1998; Stagakis et al., 2010). Spectra measured across all field sites and all VZAs did not possess standard/typical vegetation curves. Instead, vegetation reflectance curves were similar to those of other Arctic studies (e.g. Liu et al., 2017; Bratsch et al., 2016; Buchhorn et al., 2013) where visible soil/substrates and non-photosynthetic vegetation components (i.e. senescent vegetation) caused a general progressive increase in reflectance across the VIS, RE, and NIR regions. For example, VIS reflectance showed a general increase with increasing wavelength as is typical of mineral soil reflectance; the same was true for NIR reflectance, especially in the high Arctic site (i.e. Banks Island) where spectral morphology was attributable to a high degree/prevalence of gaps comprised of visible soils/substrates. RE values in low Arctic sites exhibited a greater RE slope compared to high Arctic sites. RE (and VIS and NIR) values are consistent with progressively less photosynthetic vegetation components and more visible soil per unit area at higher latitudes. Indeed, measured values of LCC and PAI_e decrease with increasing latitude as was shown in previous chapters. These are all expected general conclusions presented in previous studies. However, the comprehensive analysis presented here for multiple field sites on a latitudinal gradient, different spectral data sets (full ASD spectrum and re-sampled CHRIS M1 simulated spectra) and different spatial scales (plot and subplot) is new and provided a strong basis for the next phases of this thesis, RTM modelling at both the field and satellite imaging scales.

The detailed analysis of parametric and non-parametric techniques to determine optimal bands for VIs and to evaluate their performance in vegetation modeling over the multiple sites, view angles and spectral and spatial scales is also new.

(2) Parametric analysis of all spectral datasets using all multi-band VIs showed that the prediction of LCC, PAI_e and CCC_e was most consistent and least sensitive to angular effects when using the simple ratio (SR). The initial assessment of VIs showed that NDVI produced similar results to SR. Indeed, NDVI has been explored using all two-band combinations in other Arctic based studies with moderate to good success (e.g. Liu et al., 2017); however, there has not been a complete systematic assessment of multi-band formulations and their resistance (compensation) to angular effects caused by extreme sun-target-sensor geometry, as is typical for optical studies in the Arctic. Nor has there been an assessment of multi-band VIs for their ability to derive predictions/estimations of foliar chlorophyll quantities (LCC), effective plant area index (PAI_e), or effective canopy chlorophyll content (CCC_e) using cross-validated calibrated equations derived from multi-angle spectroscopic data. Conclusions drawn from the multi-band VI analysis conducted with the multi-angle, spectrally resampled, and spatially resampled datasets are as follows.

(i) Best estimates of LCC, PAI_e, and CCC_e were achieved at the plot scale (i.e. >1 m²). Subplot measurements at the 1 m² can be considered not spatially representative, given that all Arctic sites sampled in this study were extremely spatially diverse at the subplot scale (i.e. <1m²), even within spectrally homogeneous plant assemblages. Although the reduction of spatial variability may be important when scaling up to intermediate satellite scales, it is likely an important consideration for high spatial resolution sensors. The overall best estimates were achieved in the high Arctic where there exist greater differences between vegetation assemblages but this is not reflected to the same extent in lower latitude sites. Good results have been reported in the high Arctic using narrowband VIs (e.g. Liu et al., 2017); however, relationships reported in this study did not hold over the entirety of the sampled bioclimatic gradient, even when sampling methods remained

consistent. This result suggests that low-statured, two-dimensional, and less complex canopies produce better results because vegetation elements (i.e. leaves) are not obscured by the vertical complexity of the canopy.

(ii) A data subset using coarser spectral sampling (i.e. the M1 simulated CHRIS/PROBA, bandwidths of ~ 10 nm) produced slightly less accurate predictions as compared to the full spectrum narrow bands (< 2 nm). This outcome appears to support the notion that narrower bands provide better exploitation of subtle absorption and reflectance features of Arctic vegetation. However, the results of the predefined narrowband vegetation analysis of this study suggest that a bandwidth difference of ~ 2 to ~ 10 nm has no effect (as reported for the ROSAVI results). An explanation for better performance with the ASD dataset compared to the simulated CHRIS/PROBA M1 data may be that band centre positions for the CHRIS sensor are not in the optimal locations for detecting Arctic tundra vegetation biochemical and biophysical properties.

(iii) Optimal wavelength regions are in-line with well-known spectral absorption regions for pigments (i.e. LCC, PAI_e, and CCC_e) in the VIS (e.g. ~ 616 - 699 nm) and for their associated structural components (i.e. cell and canopy structure) in the RE and NIR (e.g. ~ 710 - 881 nm), as reported in a previous study examining Arctic green vegetation components (e.g. Liu et al., 2017). However, the large range of optimal band values reported here is directly related to (multi-angle) reflectance anisotropy; this is one of the most important results of this study. As discussed previously, there are observed reflectance differences related to observation angle, where negative view angles produce greater reflectance and nadir view angles produce the least; positive view angles produce greater reflectance values than nadir, thus causing a mixture of specular and diffuse reflectance. The SR band analysis showed that there is an average shift of approximately 100 nm in the optimal central bands when detecting all variables (LCC, PAI_e, and CCC_e, individually and

when combined into one result). Upon inspection of the field spectra, it may be obvious that there should be a systematic shift in optimal wavelengths considering the systematic reflectance differences that exist between the measured VZAs. The attenuation of radiation into vegetation is typically wavelength dependent; longer wavelengths will penetrate further into vegetation canopies, thus causing wavelength selections to shift to longer wavelengths (as it passes through a greater amount of foliage) before returning to the sensor). Although attempts were made to replicate the theoretical back/forward scatter geometries of the CHRIS/PROBA sensor, future ground-based, multi-angle spectroscopic studies should factor in the precise location of the sun. It is possible that results achieved were affected by variable solar azimuth and zenith angles.

(iv) Finally, it was shown that the optimal r^2_{cv} values obtained for all vegetation variables across all sites were achieved at -55° when using the SR and the full spectrum dataset (and the average of all four spectral datasets combined), although modelling gains were minimal over other VZAs (e.g. $r^2_{cv} \pm 0.04$). Model accuracies were best achieved at the 0° and $+55^\circ$ VZAs ($\text{NRMSE}_{cv} = 0.12$ and $\text{NRMSE}_{cv} = 0.13$, respectively); however, difference to modelling error was minimal between all VZAs ($\text{NRMSE}_{cv} \pm 0.02$). Other studies examining the effect of view angle on the estimation of bio-geophysical variables often conclude that off-nadir observations are more useful, since less background is visible within the field of view (Takebe et al., 1990). Furthermore, it is often stated that backscatter observations serve better than forward scattering for the estimation of bio-geophysical variables (Seed & King, 2003; Galvão et al., 2009; Walter-Shea et al., 1997). However, this does not always hold true. Stagakis et al. (2010) showed that the retrieval of chlorophyll, carotenoids, and leaf area index were best estimated at $+55^\circ$ within a Mediterranean ecosystem. It was further stated that at such extreme view angles background effects are minimized (i.e. gap fractions are minimized), and thus the results implied that soil background influences are

far more important than shadow effects regarding the reliability of the reflectance signal (Stagakis et al., 2010). This reasoning may also hold in the Arctic due to the low stature and density of the canopy (less overall influence of shadow); canopy gaps will inevitably lead to soil exposure. Verrelst et al. (2008) reported significant reflectance anisotropy of vegetation canopies and variable angular response of VIs in two contrasting structural vegetation types, a pine forest and meadow. They concluded that shadowing is not the driving factor, but instead the proportion of photosynthetic, non-photosynthetic and background compounds significantly affects VI values.

A final statement should be made concerning the use of brute-force assessments of optimal VI bands: this method is a very time-consuming process! It is advisable that future studies conducted with this technique do so with targeted spectral bands in meaningful spectral regions related to the biochemical and biophysical variables in question; however, the selection of bands outside of these regions may sometimes be important (as was shown with wavelength selections in the lower and upper regions of the measurements – parameter covariation). Indirect reflectance responses to biochemical constituents may play a role in the selection of bands outside of known response ranges. For example, Haboudane et al. (2004) reported that chlorophyll concentration indirectly affects the reflectance curve at infrared wavelengths, and Filella and Peñuelas (1994) stated that vegetation water content can indirectly affect red-edge reflectance. Band reduction techniques are discussed elsewhere (Verrelst et al., 2015a,b).

(3) An interesting result of the predefined narrowband VI analysis was that ROSAVI performed the best overall irrespective of VZA and vegetation variable. Soil based VIs (e.g. SAVI variants) have been extensively tested in agriculture contexts but have been applied less in vegetation modelling/retrieval testing in natural ecosystems (e.g. Wu et al., 2008). Furthermore, SAVI based VIs have been tested less in Arctic environments compared to various narrowband VIs such as

NDVI (e.g. Liu et al, 2017, Buchhorn et al., 2013), which is surprising considering the sparse canopies and overall additive influence of soils and other non-green vegetation components to Arctic tundra reflectance spectra. Of the 84 tested VIs, four SAVI based VIs were among the top ten results (ROSAVI, OSAVI, TSAVI, and RMCARI/ROSAVI). Conclusions drawn from the predefined VI analysis conducted with the multi-angle, spectrally resampled, and spatially resampled datasets are as follows. (i) Like the SR analysis, the best estimates of LCC, PAI_e, and CCC_e were achieved at the plot scale (i.e. >1 m²). Furthermore, similar regional-based results were achieved using ROSAVI. Banks Island, once again, produced the best overall predictions of LCC, PAI_e, and CCC_e compared to the other sites. (ii) The simulated CHRIS/PROBA dataset produced very similar results as the full spectrum ASD dataset at both spatial scales. (iii) Wavelengths used in ROSAVI (705 and 750) are within the realm of meaningful spectral bands chosen in the multi-band analysis; however, they are not optimal for the Arctic as is evident from the poorer results of the analysis. It is possible that the ROSAVI formulation explored through a multiband analysis has the potential to outcompete SR. (iv) It was shown that the optimal r^2_{cv} values obtained for all vegetation variables across all sites were achieved at -55° when using the ROSAVI, although modeling gains were minimal over other VZAs (e.g. $r^2_{cv} \pm 0.04$). Model accuracies were best achieved at the -55° and +55° VZAs (NRMSE_{cv}=0.16 and NRMSE_{cv}=0.15, respectively); however, it should be noted that difference in modelling error was once again minimal between all VZAs (NRMSE_{cv}±0.03). The largest benefit of using predefined indices is their processing speeds, which was found to be almost instantaneous.

(4) Gaussian Processes Regression (GPR) was shown to produce the overall best r^2_{cv} based results with the simulated CHRIS/PROBA M1 dataset, although, results were comparable to those obtained using the multi-band SR (r^2_{cv} =0.62 vs. r^2_{cv} =0.58, respectively). Overall, it was shown

that GPR had a slightly lower mean predictive capability than SR ($\text{NRMSE}_{cv}=0.16$ and $\text{NRMSE}_{cv}=0.12$, respectively), but produced equivalent predictions to ROSAVI. Full spectrum methods have seldom been used for biophysical or biochemical retrievals in Arctic environments and additionally have not been tested for spectroscopic retrievals of LCC, PAI_e , or CCC_e using multi-angle spectroscopic data. Conclusions drawn from the GPR analysis conducted with the multi-angle, spectrally resampled, and spatially resampled datasets are as follows.

(i) Like the previous analyses, the best estimates of LCC, PAI_e , and CCC_e were achieved at the plot scale (i.e. $>1 \text{ m}^2$). Furthermore, similar regional based results were achieved; Banks Island produced the best overall predictions of LCC, PAI_e , and CCC_e .

(ii) The use of all narrow spectral bands led to suboptimal regression performance, as was reported elsewhere (Verrelst et al., 2016). Generally, entering all spectroscopic (i.e. hyperspectral) bands into a regression model is not an ideal approach due to multi-collinearity and inclusion of noisy bands (Verrelst et al., 2016). To overcome this problem, it is recommended to use band selection based on expert knowledge or to use spectral reduction techniques (e.g. principal component analysis). In this study, the reduction of the full spectrum spectroscopic dataset was based on the CHRIS/PROBA Mode-1 band set, which uses approximately 62 bands ranging from 411 to 997 nm and with spectral bandwidths of approximately 10 nm. This reduction of variables ultimately led to enhanced results over full spectrum narrowband data (i.e. 2 nm vs. 10 nm). Mapping variables with broader bands has been demonstrated. For instance, Kira et al. (2016) showed that 2 nm bandwidth data resampled to 10 nm resolution were adequate in their representation of the original data (i.e. minimized loss of data content) while greatly increasing the processing time (they used neural networks and partial least squares regression). Furthermore, Verrelst et al. (2016) showed that optimal results can be achieved with as little as four HyMap

bands for retrieving LAI. What is interesting here is that these results are contrasted with narrow bands being more beneficial for multiband VI retrievals. GPR testing conducted by Verrelst et al. (2016) showed that band redundancy is less an issue when using super-spectral data (typically <50 bands) and that results obtained with such data can lead to top-performing regression models. What is of utmost importance, however, is the placement of the spectral bands along the spectral range, as was demonstrated with the SR and ROSAVI analysis. Waveband performance for vegetation analysis applications has been assessed in other studies (e.g. Thenkabail et al., 2004).

(iii) For each of the variables (LCC, PAI_e, and CCC_e), bands within the chlorophyll absorption region (~675 nm) and the red-edge reflectance regions (~720 nm) were found to be crucial for retrievals. In these regions both pigment concentrations and vegetation structural attributes govern canopy reflectance. The importance of these regions has been demonstrated in other Arctic based studies (e.g. Liu et al., 2017; Buchhorn et al., 2013; Bratsch et al., 2016). Accordingly, GPR results demonstrate that band selections are physically meaningful at all VZAs (which has implications for the modelling conducted with multi-angle CHRIS data in Chapter 6) and across all sites. Another aspect to be considered when analyzing relevant bands is the signal-to-noise-ratio of the sensor (spectroradiometer or imaging spectrometer). VIS-NIR spectroradiometers typically use silicon photodiode detectors that are characterized by a decreasing signal-to-noise at the shortest (<450 nm) and longest (>900 nm) wavelengths (Milton et al., 2009). As identified by (Verrelst et al., 2016), irregular high and low l_b values, and thus band selections, in these regions may be due to poor SNR, rather than information content related to vegetation properties. The spectral shift that was detected in the multi-band SR analysis was not as significant in the GPR analysis. When examining the simulated CHRIS/PROBA dataset, a very slight increase in optimal wavelength

regions (averaged across all variables) are detectable when progressing from negative to positive VZAs (Figure 60, top left).

(iv) Finally, it was shown that the optimal r^2_{cv} values obtained for all vegetation variables across all sites were achieved at -55° when using GPR in combination with the simulated CHRIS/PROBA dataset (at both plot and subplot scales); however, best prediction accuracies were achieved at the 0° and -36° VZAs ($\text{NRMSE}_{cv}=0.15$ for both). It is possible that backscatter reflectance is optimal for retrieving biochemical and biophysical vegetation variables due to the lack of shadows (i.e. obscured canopy components – the canopy view is maximized); however, analysis of model accuracies does not fully support this. As previously stated, model accuracies were very similar for all VZAs ($\text{NRMSE}_{cv}\pm 0.02$).

(5) Overall conclusions drawn from this study and applied to later Chapters are as follows. (i) The simple ratio (SR) and revised optimized soil adjusted vegetation index (ROSAVI) were determined to be the optimal multi-band and predefined multi-angle VIs, respectively. Although soil-based VIs produced favorably in the predefined narrowband VI comparison, the SR produced better modelling outcomes than the multi-band SAVI. The VI analyses conducted at the remote sensing scale employ the SR and ROSAVI VIs. (ii) The GPR algorithm produced favorable results when used in combination with a spectrally reduced dataset (i.e. CHRIS M1). Furthermore, GPR model run time was not considered a deterrent for use with a 1-band removal iteration procedure; all subsequent GPR modelling was conducted using this procedure. (iii) The optimal multi-angle spectral regions for variable retrievals (LCC , PAI_e , and CCC_e) were revealed to be largely within 450-550 nm and 650-750 nm; however, due to the large degree variable covariation observed in the band selections across all VZAs, the choice was made to continue further analyses using the original spectral dimensionality of the two sensors employed in this study (ASD and

CHRIS/PROBA). (iv) Modelling accuracies were best achieved at the plot scale ($>1 \text{ m}^2$) across all model types, vegetation variables, and view angles. A reduction in subplot variability was determined to be a necessary procedure for increasing model outcomes (i.e. r^2 , RMSE, NRMSE). All subsequent modelling, inclusive of the radiative transfer modelling in Chapter 6, was conducted at the plot scale.

Chapter 6. Evaluation of a Physical Modelling and Inversion Retrieval Method for Predicting Vegetation Biochemical and Biophysical Variables Across an Arctic Bioclimatic Gradient

Abstract

Vegetation monitoring in Arctic regions has been mostly accomplished through classification and empirically-based biophysical variable estimation with nadir looking broadband instruments at coarse spatial scales. Recent advances in multi-angle, high spatial resolution imaging spectroscopy (e.g. CHRIS/PROBA) present a significant opportunity to improve retrievals of biochemical and biophysical vegetation properties using physically-based modelling approaches that have yet to be investigated in Arctic ecosystems. Such instruments (and future spectroscopic instruments, such as EnMap) also provide a unique platform from which to test directionally-based leaf and canopy physical models (i.e. PROSAIL). In this study, field-based vegetation modelling was conducted to develop understanding and methods for subsequent satellite-based modelling to be presented in Ch. 7. The PROSAIL leaf and canopy radiative transfer model (RTM) was inverted using a numerical iterative optimization approach (Levenberg-Marquardt algorithm, LMA) to extract leaf-canopy biochemical (i.e. leaf chlorophyll content, LCC and effective canopy chlorophyll content, CCC_e) and biophysical (i.e. effective plant area index, PAI_e) parameters and variables from multi-angle, ground-based spectroradiometry. PROSAIL inversions were investigated using two spectral datasets: multi-angle full spectrum data, and simulated CHRIS/PROBA (411-997 nm) spectra. Multi-angle spectral measurements, equal to the view zenith angles (VZAs) acquired by CHRIS/PROBA (-55°, -36°, 0°, +36°, +55°), and biochemical-biophysical measurements were collected between the years 2011 to 2014 across a bioclimatic gradient in the Western Canadian Arctic. PROSAIL model parameters were constrained using the

measured and modelled field variables (i.e. chlorophyll, carotenoids, equivalent water thickness, dry leaf matter, leaf area index, and leaf angle distribution) and known sun-target-sensor geometry. Additional leaf and canopy model parameters were constrained with accepted published values. Overall, it was shown that PROSAIL could simulate the multi-angle top-of-canopy spectral reflectance of Arctic canopies ($r^2 \sim 0.99$, RMSE=0.004 $\pm$ 0.002); however, it was not capable of accurately modelling LCC, PAI_e, and CCC_e across a diversity of field sites (mean combined inversion results of all sites, VZAs, and vegetation variables $r^2=0.31$, NRMSE=0.30). The results for the full spectrum dataset demonstrated that the PROSAIL and the LMA inversion approach have the capability of modelling biochemical and biophysical variables in sparsely vegetated high Arctic sites when compared against the validation dataset (LCC $r^2=0.76$, RMSE=9.94; PAI_e $r^2=0.64$, RMSE=0.64; CCC_e, $r^2=0.79$, RMSE=0.12); however, predictions demonstrate a strong positive bias. Overall results for the full spectrum dataset when taken across combined vegetation variables, field sites, and VZAs produced a mean correlation of $r^2=0.33$ with a mean NRMSE=0.32, whereas the use of a spectral subset (CHRIS/PROBA M1) led to overall poorer relationships ($r^2=0.28$), though model predictions improved (NRMSE=0.29). Averaged results across all sites and datasets showed that the best predicted vegetation variable was the CCC_e ($r^2=0.33$, NRMSE=0.24), followed by the LCC ($r^2=0.32$, NRMSE=0.28) and PAI_e ($r^2=0.28$, NRMSE=0.40). The overall best performing VZA across all field sites and vegetation variables was 0° ($r^2=0.44$, NRMSE=0.28) followed by +55° ($r^2=0.39$, NRMSE=0.30); however, results were not considerably different than the other VZAs. Conclusions drawn from this study are that future modelling efforts should focus on the evaluation of RTMs suitable for three-dimensional heterogeneous canopies and further investigate various robust inversion methodologies and regularization strategies.

6.1. Introduction

Quantitative retrieval of vegetation biochemical and biophysical characteristics from optical remote sensing data is the basis for a variety of ecological monitoring applications (Stow et al., 2004; Ustin et al., 2004; Ustin et al., 2009; Kokaly et al., 2009; Jacquemoud et al., 2009; Hilker et al., 2012; Verrelst et al., 2015a,b; Croft et al., 2014; Croft et al., 2015; Clevers et al., 2017). Imaging spectrometers are enabling enhanced detection/retrieval and monitoring capabilities for plant variables, such as foliar and canopy level pigments (e.g. leaf and canopy chlorophyll content) and canopy structure (e.g. leaf area index) (Bacour et al., 2006; Houborg et al., 2007; Moulin et al., 1998; Dorigo et al., 2007; Darvishzadeh et al., 2008a; Stagakis et al., 2010; Sykioti et al., 2011; Verrelst et al., 2015a). Leaf area index (LAI), a key variable within ecological research and monitoring (Watson, 1947; Boelman et al. 2003, Breda 2003, Ewert 2004, Van Wijk et al. 2005; Mougin et al., 2014), has been linked to atmosphere-vegetation exchange processes, such as photosynthesis, evapotranspiration, and carbon flux (Soegaard, 1999; Leuning et al., 2005; Duchemin, et al., 2006; Cleugh et al., 2007; Jongschaap, 2006; Chen et al., 2006; Chen et al., 2007; Zheng & Moskal, 2009). Quantitative estimates of LAI can provide an understanding of dynamic changes in ecosystem productivity and offer a metric for which climate related impacts to ecosystems can be assessed (Zheng & Moskal, 2009; Green et al., 1997; Liu et al., 1997). Leaf chlorophyll content (LCC) and synthetic variables such as canopy chlorophyll content (CCC, defined as the product of LAI and LCC) contribute to the assessment of vegetation physiological status and health, and have been found useful for detecting vegetation stress, photosynthetic capacity, and productivity across ecosystems (Blackburn et al, 1998a; Gitelson et al., 2005; Darvishzadeh et al., 2008a; Yin et al., 2016; Croft et al., 2014; Verrelst et al., 2015a; Peng et al., 2017; Clevers et al., 2017).

Retrieval of vegetation variables from optical remote sensing data may be conducted using empirical or physically-based methods. Empirical modelling is used to establish correlations between parameterized expressions (i.e. vegetation indices, VIs) and measured biochemical and biophysical vegetation variables (Croft et al., 2014; Verrelst et al., 2015a,b; Verrelst et al., 2016; Liu et al., 2017). Empirical methods (both parametric and non-parametric) have been shown to produce excellent results in a variety of environments (e.g. Croft et al., 2014; Verrelst et al., 2015a,b; Verrelst et al., 2016; Liu et al., 2017; Clevers et al., 2017), while providing a rather simple and straightforward approach for implementation. Two limitations related to their use are: (1) parameterized empirical models may not be transferrable to new locations as they typically require recalibration, and (2) empirical models can suffer from statistical problems such as overfitting (Darvishzadeh et al., 2008a; Verrelst et al., 2015a,b; Verrelst et al., 2016). On the other hand, physical radiative transfer models (RTMs) models used in optical remote sensing, describe the interaction (absorption, scattering and reflectance) of radiation within a medium, typically leaves and their associated canopies using physical laws (mathematical expressions), and are thus considered generalizable across ecosystems (Jacquemoud et al., 2009). Leaf and canopy RTMs, such as PROSAIL (PROSPECT (leaf) + SAIL (canopy)) (Jacquemoud & Baret, 1990; Verhoef, 1984; Verhoef, 1985; Feret et al., 2008; Jacquemoud et al., 2009), assume that radiative transfer and interaction of radiation within leaves and canopies is a function of leaf structure and biochemistry, canopy architecture/configuration, and soil characteristics (e.g. moisture and composition) (Darvishzadeh et al., 2008a; Feret et al., 2008; Jacquemoud et al., 2009; Feret et al., 2017). They therefore provide an explicit connection/link between vegetation biophysical and biochemical variables and canopy directional and hemispherical reflectance (Jacquemoud et al., 2009). PROSAIL provides a means to generate top-of-canopy (TOC) spectral databases, which

can be used to test new spectral indices, or perform model sensitivity analyses to identify the causal mechanisms influencing reflectance (Jacquemoud et al., 2009). In addition, PROSAIL has been widely used to estimate biophysical and biochemical attributes of canopies as it relates to multi-angle reflectance data (e.g. Botha et al., 2007; Verrelst et al., 2008; Verrelst et al., 2010; Hilker et al., 2011; Liang et al., 2015; Hilker et al., 2017); however, the PROSAIL RTM has not been tested in Arctic environments to estimate biochemical or biophysical attributes of tundra vegetation using multi-angle spectroscopic data. PROSAIL has been successfully used in ecosystems such as grasslands to estimate leaf chlorophyll, leaf area, and canopy chlorophyll content (Darvishzadeh et al., 2008a,b). Therefore, investigating its potential in a similar low-stature ecosystem is warranted.

To be able to use PROSAIL for the retrieval of vegetation characteristics from measured reflectance data, it must be inverted (Kimes et al., 2000; Jacquemoud et al., 2009). The inversion of PROSAIL with remote sensing or field-based spectroradiometer data is considered a physically sound approach for the retrieval of biophysical and biochemical variables since the approach is generic, and therefore (in theory) applicable across ecosystems (Dorigo et al., 2007; Jacquemoud et al., 2009; Verrelts et al, 2015). Despite the perceived simplicity of RTMs such as PROSAIL (i.e. it is a generalization of a physical system), inversion is not straightforward due to the inherent complexity of the combined leaf-canopy models (i.e. the number of variables) and the intricacy involved with running the model in reverse (i.e. the choice of method used for inversion). Furthermore, the inversion of RTMs is mostly under-determined and ill-posed; the number of unknowns is typically much larger than the number of independent observations, and furthermore, various combinations of input parameters may result in the same solution (Verrelst et al., 2015a,b; Jacquemoud et al., 2009). These properties of the physically-based approach, within the remote

sensing framework, make physically-based retrievals of vegetation properties a challenging task. To help overcome this problem, some restrictions/regularizations on the inversion process can be implemented to constrain the inversion process. For example, the use of prior knowledge about model parameters (e.g. measured variables in the field) or accepted values can be used (Botha et al., 2007; Darvishzadeh et al., 2008a; Verrelst et al., 2015a,b).

Iterative optimization, or curve fitting, is a common technique used to invert leaf and canopy RTMs (Jacquemoud et al., 2009; Vohland et al., 2010; Liang et al., 2015; Verrelst et al., 2015b; Hilker et al., 2017; Feret et al., 2008; Feret et al., 2017). It consists of the minimization of a cost function which estimates (quantifies) the difference between the measured and estimated variables (i.e. the measured and modelled spectra) by successively iterating the parameters of the RTM until the spectral curves match as closely as possible (i.e. the value of the merit function is minimized). The model parameter combination that makes up the solution to the matched spectra is considered the starting point, and thus could be considered the inverted parameters. Drawbacks of using optimization techniques in an operational setting are that (1) regularization techniques are required to achieve accurate results (Zarco-Tejada et al., 2001; Verrelst et al., 2015b), however, this can be expected when using any inversion technique such as look-up-tables (LUT) (e.g. constraining variables from field measurements or expected values, the use of multiple best solutions, etc.); and (2) inversion is sensitive to the model's initial input parameters (e.g. initial values may contribute to curve fitting algorithms getting caught in local minima before reaching global minima) (Liang, 2005; Verger et al., 2011). Another downside to using numerical optimization is that the technique is computationally demanding, a severe limitation that makes retrieval across broad geographic areas unrealistic (e.g. when used to process each pixel in a remote sensing image, and when many spectral bands are used). Despite these drawbacks, numerical optimization methods can serve as a

preliminary means of testing RTMs across previously untested terrain/ecosystems or serve as a means of determining parameter ranges not measurable in the field (and that would otherwise be a guess when implementing other inversion methods such as LUTs or artificial neural networks [ANN] approaches).

Common numerical optimization algorithms used to invert RTMs include the Nelder-Mead downhill simplex algorithm (Nelder & Mead, 1965), the quasi-Newton method (Gauss-Newton) (Meroni et al., 2004), and the Levenberg-Marquardt algorithm (LMA) (Levenberg, 1944; Marquardt, 1963; Morrison, 1960). Each have been used in various studies with various levels of success (e.g. Vohland et al., 2010; Hilker et al., 2017). Comparative studies examining inversion techniques with PROSAIL are rather limited (Sehgal et al., 2016); however, several studies have been conducted comparing numerical optimization to LUTs and ANNs. A study conducted by Vohland et al. (2010) compared numerical optimization (downhill simplex method) to LUTs and ANNs for inverting PROSAIL, and results showed that numerical optimization could outcompete the other methods for estimating vegetation variables. Preidl and Doktor (2011) demonstrated that a quasi-newton numeric optimization was capable of outperforming LUT and support vector regression inversion techniques. Hilker et al. (2017) used the LMA method for inverting the PROSAIL model with multi-angle Moderate Resolution Imaging Spectroscopy (MODIS) to estimate vegetation chlorophyll quantities in the Amazon Rainforest, and showed that LMA inversion can produce excellent results when compared to measured chlorophyll values (up to $r^2=0.98$). To date, there have been no attempts at inverting PROSAIL for the estimation of biochemical or biophysical vegetation properties in heterogeneous Arctic environments using spectroscopic data, but there are numerous empirical studies (Liu et al., 2017; Brtasch et al., 2016; Buchhorn et al., 2013). Considering the success of the LMA optimized inversion used by Hilker

et al. (2017), the goal here is to evaluate the use of the LMA numerical optimization for inversion of multi-angle spectroscopic field data to estimate leaf chlorophyll content (LCC), effective plant area index (PAI_e, as previously defined in Chapter 4), and effective canopy chlorophyll content (CCC_e, as previously defined in Chapter 4). Lastly, most studies using PROSAIL have not been done across multiple field sites or ecological gradients to test its generalizability, as presented here.

Considering the above, the primary objective of this study was to estimate and predict measured LCC, PAI_e, and CCC_e of Arctic tundra vegetation by inverting the PROSAIL RTM with multi-angle field-scale spectroscopic data. The secondary objective was to test the capability of the Levenberg-Marquardt numerical optimization inversion algorithm for predicting LCC, PAI_e, and CCC_e at various sun-target-sensor geometries and across a latitudinal gradient in the Western Canadian Arctic, thus testing the general applicability of the method under a wide variety of typical remote sensing conditions. A sub-objective here was to estimate average leaf and canopy variable values through the inversion of the PROSAIL model that could be applied to the CHRIS/PROBA satellite-based remote sensing analysis presented in Chapter 7 (i.e. determination of optimal parameter starting values and constraints). The final objective of the study was to test the effect of varying the spectral resolution on the prediction of field-based measurements (i.e. down-sampling the spectral data to match those of the CHRIS/PROBA sensor (Barnsley et al., 2004) to understand the effect of spectral scale on multi-angle retrievals of biochemical and biophysical parameters (i.e. does band-width matter?).

6.2. Materials and Methods

6.2.1. Study sites

The study areas used for the field scale physical analysis were based on the field locations detailed earlier in the thesis (Chapter 5). All field sites were visited between July 10th and August

4th in given years between 2011 and 2014 during what is considered the peak of the growing seasons to minimize any phenological variability introduced by the short tundra growing season. Table 23 (Chapter 5, Section 5.2.2.) shows the date and time range that each location was sampled.

6.2.2. Ground data and spectral measurements

Field-sample design and measurements of leaf chlorophyll content (LCC, $\mu\text{g}/\text{cm}^2$), leaf area index (effective plant area index, PAI_e , m^2/m^2 , hereafter), canopy chlorophyll content (effective canopy chlorophyll content, CCC_e , g/m^2 , hereafter), and multi-angle field spectra were described previously in Chapter 5. An in-depth description of the LCC sampling and processing can be found in Chapter 3. The description of the measurement and modelling of PAI_e can be found in Chapter 4. Description of the field-based multi-angle spectral sampling can be found in Chapter 5. The sun-target-sensor geometry shown in Table 23 (Chapter 5, Section 5.2.2.) was used to parameterize the PROSAIL RTM at each site; spectra time stamps were used to determine exact sun/sensor geometry. All sample sizes (for all measured variables) are consistent with previous chapters.

Spectral datasets used in the analysis were the ASD full spectrum narrowband dataset ($\sim 2\text{nm}$ spectral resolution) and the simulated CHRIS/PROBA M1 dataset ($\sim 10\text{nm}$ spectral resolution) as described in Chapter 5 (Section 5.2.2.). Noisy spectral bands were discarded from the dataset, ultimately leading to spectral dataset extending from 400 to 1050 nm and 411 to 997 nm, respectively. Weiss et al. (2000) found that the accuracy of model estimation worsens when the spectral range is high (e.g. 400 to 2500 nm); therefore, the spectral range of the datasets used in this study can be considered more appropriate. For example, the PROSAIL model is sensitive to changes in chlorophyll content in the 400–900 nm range while LAI primarily influences the red-edge (RE) and near-infrared (NIR) portions of the selected range (Guyot et al., 1992).

Within each of the measured subplots, vegetation species composition and relative abundance showed the same general degree of variability (i.e. all subplots were heterogeneous at the 1 m² scale). Species varied in terms of leaf shape, leaf size, and the amount of leaves (i.e. PAI_e) and the distribution of their typical average leaf angles (ALA); therefore, all foliar measurements (e.g. LCC) and modelled canopy values (e.g. ALA) represent the average conditions within each of the subplots. Destructive measurements of foliar and canopy carotenoid content, equivalent water thickness (EWT), and dry matter content (leaf dry mass) acquired in the Richardson Mountains during the 2014 field season (see Chapter 3, Section 3.3.2.) were used as modelling values across all sites, as dominant vegetation types remained (to a certain extent) consistent between sites. Because optimal results in the empirical modelling study of Chapter 5 were achieved at the plot scale, all physical modelling in this study was also conducted at the plot scale (i.e. subplots averaged into plots; spatial resampling described in Chapter 5).

6.2.3. Physical modelling: *PROSPECT+SAIL (PROSAIL)*

The PROSAIL RTM (Jacquemoud et al., 2009), an amalgamation of the PROSPECT-5 leaf optical properties model (Jacquemoud & Baret, 1990; Feret et al., 2008) and the SAILH canopy bidirectional reflectance model (Verhoef, 1984; Verhoef, 1985; Kuusk, 1991), was used to simulate TOC spectral reflectance and retrieve LCC, PAI_e, and CCC_e at all field sites. Both models are moderately straightforward representations of leaves and canopies and require a limited number of input parameters (six and eight, respectively). Through the inversion of PROSAIL, both leaf and canopy parameters can be estimated/predicted from measured TOC spectral reflectance.

The PROSPECT-5 model calculates the directional-hemispherical reflectance and transmittance of leaves based on two classes of input variables: (1) the leaf structure parameter (N) which is the number of compact layers specifying the average number of air/cell wall interfaces

within the mesophyll; and (2) the leaf biochemical content (total chlorophylls, C_{ab} ; total carotenoids, C_{ar} ; brown pigment content, C_{bp} ; equivalent water thickness, C_w ; dry matter content, C_m) (Jacquemoud et al., 2009). The PROSPECT-5 model parameters are shown in Table 33 with their respective units. Unlike the PROSPECT-4 model, PROSPECT-5 does not uniformly treat all photosynthetic pigments (chlorophylls and carotenoids) as entirely chlorophyll (Feret et al., 2008). The newest version of PROSPECT, PROSPECT-D (D is for dynamic), which includes anthocyanins, was not used in the research because of its recent release (Feret et al., 2017). The spectral leaf optical properties (reflectance and transmittance) calculated by PROSPECT-5 are inputs into the SAILH canopy reflectance model.

SAIL simulates the bidirectional reflectance factor (BRF) of turbid-medium plant canopies (Jacquemoud et al., 2009). Defining a canopy as a turbid medium represents it as a horizontally homogenous and semi-infinite layer comprised of small vegetation elements of a given geometry and density that act as absorbing and scattering particles (Darvishzadeh et al., 2008a; Jacquemoud et al., 2009). Consequently, the model is best adopted for use in homogeneous vegetation canopies (Meroni et al., 2004; Schlerf & Atzberger, 2006; Verhoef, 1984; Darvishzadeh et al., 2008a,b). The original SAIL model considers the effect of canopy structural and optical properties while accounting for the inclination distribution of canopy elements (i.e. foliage). The SAIL RTM was later adapted/modified into the SAILH model which considers the hot spot effect in plant canopy reflectance (Verhoef, 1984; Verhoef, 1985; Kuusk, 1991). Apart from leaf reflectance and transmittance, SAILH requires eight input parameters to produce TOC hemispherical and directional reflectance simulations. It should be noted that to correctly parameterize the SAILH model, multi-angular spectral measurements need to be considered (i.e. sun/sensor geometry). SAILH parameters include: (1) leaf area index (LAI/PAI); (2) mean leaf inclination angle, (ALA);

(3) hot spot size parameter (S_L), defined as the ratio between the average size of the leaves and the canopy height (Verhoef, 1985); (4) background/soil reflectance (P_S); (5) fraction of diffuse incoming solar radiation ($SKYL$); (6) sun zenith angle (SZA); (7) sensor view zenith angle (VZA); and (8) relative azimuth angle (RAA), which is defined as the relative angle between the sun azimuth and sensor azimuth angles. Therefore, when PROSPECT-5 and SAILH are coupled into PROSAIL, these 14 input parameters pertaining to the leaf, canopy, and soil characteristics must be specified.

A simple sensitivity analysis of the PROSAIL RTM was conducted to determine the effects of varying the input parameters on simulated spectra. Tests were conducted by simultaneously iterating two PROSAIL parameters while holding all others constant; all parameters were iterated in combination with various VZAs (in accordance with the CHRIS/PROBA look angles). The results of this test are reported in Appendix D. This simple sensitivity analysis showed that sensor look angle (VZA) has a large influence on observed TOC spectral-directional reflectance in all regions of the spectrum used in this research (i.e. 400 nm to 1000 nm). Thus, the spectral-directional considerations made in the measurement and modelling of spectra are well justified.

6.2.4. Inversion based on numerical optimization: Levenberg-Marquardt algorithm (LMA)

The inversion of PROSAIL was accomplished with the Levenberg-Marquardt iterative numerical optimization algorithm (LMA) (see Chapter 2, Section 2.2.3.). The LMA was implemented through the MPFIT package for ENVI (Markwardt, 2009). MPFIT functions permit the fixing of any function parameters, as well as the ability to set simple upper and lower parameter bounds (Markwardt, 2009). Iterative optimization was chosen for this study because it is a widely used and accepted method for model inversion (Botha et al, 2007; Feret et al., 2008; Jacquemoud et al., 2009; Hilker et al., 2017; Verrelst et al., 2016; Feret et al., 2017 etc.), and moreover, it does

not require a training/calibration dataset (Combal et al., 2002; Combal et al., 2003; Botha et al., 2007). LMA was chosen because it has been shown to converge quickly (Gavin, 2017), and has recently produced excellent results with PROSAIL inversion for the retrieval of chlorophyll from multi-angle spectroscopic data (Hilker et al 2017).

In this study, LMA was used for the minimization of the cost function (i.e. merit function or divergence measure). The cost function, as it was implemented here, quantifies the difference between the measured and modelled TOC spectral-directional reflectance (Rivera et al., 2013). There are many different cost functions used for minimization problems (see Rivera et al., 2013; Leonenko et al., 2013a,b); however, it has been shown that substitution of the cost functions does not necessarily lead to increased inversion performance (Rivera et al., 2013; Verrelst et al., 2014). The cost function used to minimize the divergence between the measured and simulated spectra was the Pearson chi-square (Equation 22):

$$D[P, Q] = \sum_{\lambda_l=1}^{\lambda_n} \frac{(q(\lambda_l) - p(\lambda_l))^2}{p(\lambda_l)} \quad (22)$$

where $D[P, Q]$ represents the two functions, $P = p(\lambda_1), \dots, p(\lambda_n)$ is the measured spectral reflectance and $Q = q(\lambda_1), \dots, q(\lambda_n)$ is the corresponding simulated spectral reflectance, and $\lambda_1, \dots, \lambda_n$ represents n bands (Rivera et al., 2013). The LMA was implemented to successively iterate the PROSAIL parameters (i.e. 5000 times) until the simulated spectral curves matched as closely as possible the measured spectral curves (i.e. the value of the cost function was minimized for each plot). The PROSAIL parameter combination that made up the best solution to the matched spectra was considered the starting point, and thus considered the inverted parameters.

Drawbacks of using optimization techniques in an operational setting are that (1) regularization techniques are required to achieve accurate results (Zarco-Tejada et al., 2001; Darvishzadeh et al., 2008a,b; Verrelst et al., 2015b), however, this can be expected when using any inversion technique such as LUT (e.g. constraining the model parameters from field measurements or expected/typical values); and (2) numerical inversion is sensitive to the model's initial input parameters, given that initial values may contribute to the algorithm getting caught in local minima before reaching global minima (Botha et al., 2007). These two issues were handled in the following ways: (1) The MPIFT implementation of LMA permits the fixing of any of the fourteen PROSAIL parameters, as well as the ability to set simple upper and lower parameter bounds. Known values such as VZA, SZA, and RAA, because they are always known and unique values, were fixed for each of the model inversions. Parameters that had a known range (i.e. they were measured) were constrained by setting the upper and lower limits of the investigated/known distribution (i.e. min and max values). Table 33 shows the upper and lower boundaries for each of the PROSAIL parameters. (2) Curve fitting algorithms will converge to different local minima depending on the values used for the initial guess, the degree of noise in the measurement, and algorithm parameters (Gavin, 2017). It has been stated that it is appropriate to use the best initial guess/estimate of the starting parameters when conducting iterative curve fitting, as opposed to using an intentionally poor estimate (i.e. giving zero or maximum values when it is known that they will not occur) (Gavin, 2017). Generating random initial conditions can also minimize this problem, as well as ill-posedness (Combal et al., 2002; Combal et al., 2003; Botha et al., 2007); however, this was not done in this study.

The initial input parameters used for the inversion were based upon the statistical mean values for each of the measured field variables across all sites (Table 33). Unknown parameter values (N ,

C_{bp} , S_L , P_S , $SKYL$) were based upon accepted values found within the literature. For the leaf-structural parameter (N) of PROSPECT-5, Haboudane et al. (2004) and Houborg et al. (2007) used a fixed value of 1.55 for various crops (corn, soybean, wheat and spring barley). Jacquemoud et al. (2000) used a fixed value of $N = 1.7$ for soybean. Atzberger et al. (2003a,b) used a range of 2 ± 0.34 for wheat crops. Darvishzadeh et al. (2008a), used a range from 1.5 to 1.9 for heterogeneous grasslands. Because of the large amount of grasses and thicker leaves found in Arctic tundra environments, an initial guess of 2.0 with a range between 0.001 and 2.5 was assumed valid. For the brown pigment content (C_{bp}), Zhang et al. (2005) found that model inversion for a broad-leaf deciduous forest produced values of approximately 0.7 ± 0.25 . Verger et al. (2011) used values between 0 and 1.5 for various agricultural crops. Considering these studies as a rough guide, an initial start value 1.0 and a parameter range between 0.001 to 2.0 was used for brown pigment content. The hotspot size (S_L) and soil brightness parameter (P_S) ranges in Darvishzadeh et al. (2008a) for heterogeneous grassland (0.05 to 0.1 and 0.5 and 1.5, respectively) were used as a basis for this study and a starting value of 0.075 was selected for S_L and a starting value of 0.5 was used for P_S . For the fraction of diffuse incoming solar radiation ($SKYL$), Darvishzadeh et al. (2008a) used a value of 0.1, which is also a value used by many other studies (Cho, 2007; Schlerf and Atzberger, 2006; Verrelst et al., 2015a). In this study, a value of 0.1 was used as the start value; however, a range of 0.001 to 100.0 was implemented; a large range can be justified by the fact that $SKYL$ has only a small influence on canopy reflectance and that low SZAs are normally encountered in the Arctic (see sensitivity analysis in Appendix D) (Clevers and Verhoef, 1991).

Inverted PROSAIL TOC spectral reflectance and leaf and canopy parameter inversions were compared to measured field variables (spectra, LCC, PAI_e , and CCC_e) using the coefficient of determination (r^2) and the root mean square error (RMSE) as previously defined in this thesis.

Finally, the overall combined modelling results/predictions were compared using the normalized RMSE (NRMSE), as previously defined in this thesis.

Table 33 PROSAIL parameters used to constrain the data simulations and numerical inversion. Values that were held constant (fixed) for the model inversions are indicated with an asterisk. Values indicated with ' are based on the literature. Unitless values are of no dimension.

<i>Model</i>	<i>Symbol</i>	<i>Definition</i>	<i>Units</i>	<i>Range</i>	<i>Start</i>
PROSPECT-5	N'	Leaf structure parameter (mesophyll)	Unitless	0.001 – 2.5	1.5
	C_{ab}/LCC	Chlorophyll $a+b$ content	$\mu\text{g}/\text{cm}^{-2}$	0.001 – 55.0	30.0
	C_{ar}	Carotenoid content	$\mu\text{g}/\text{cm}^{-2}$	0.001 – 25.0	12.0
	C_{bp}'	Brown pigment content	Unitless	0.001 – 2.0	1.0
	C_w	Equivalent water thickness	g/cm^{-2}	0.001 – 0.08	0.003
	C_m	Dry matter content (leaf mass per area)	g/cm^{-2}	0.001 – 0.05	0.03
SAILH	LAI/PAI_e	Leaf area index/plant area index	$\text{m}^2 \text{ m}^{-2}$	0.001 – 2.5	1.0
	ALA	Average leaf angle	Deg	$0.0^\circ - 80.0^\circ$	45.0
	S_L'	Hot spot parameter	m m^{-1}	0.05 – 0.1	0.075
	P_s'	Soil reflectance assumed Lambertian or not	Unitless	0.001 – 1.5	0.5
	$SKYL'$	Ratio of diffuse to total incident radiation	Unitless	0.001 – 100.0	0.1
	SZA^*	Solar zenith angle	Deg	$40.0^\circ - 66.0^\circ$	-
	VZA^*	Viewing zenith angle	Deg	$-55.0^\circ - 55.0^\circ$	-
	RAA^*	Relative azimuth angle (between sun/sensor)	Deg	$0.01^\circ - 180.0^\circ$	-

6.3. Results

6.3.1. Inversion of the ASD and M1 spectral reflectance datasets: Curve fitting validation

The curve fitting performance of the LMA inversion was judged using the r^2 and the RMSE between the measured and estimated spectra. Figure 61 shows the results for various VZAs and field sites. Inverted modelled parameters are shown for each curve. In the examples shown, the simulated directional-reflectance spectra were in good agreement with the field measured TOC reflectance values ($r^2 \sim 0.99$, $\text{RMSE} = 0.004 \pm 0.002$). The curve fitting algorithm was capable of reproducing TOC directional-reflectance for all value ranges of LCC, PAI_e , and CCC_e , (i.e. low to high values) and at all VZAs (a range of values is shown in Figure 61, with similar results as those

shown). The initial parameter values (Table 33) used for the analysis did not result in the algorithm getting stuck in local minima; however, as expected, experimentation with setting initial parameters to zero did. This supports the notion that providing the best possible guess for model start values is appropriate practice when using numerical optimization inversion (Gavin, 2017). Further experimentation with allowable iterations showed that optimum curve fitting results were achieved with more than 100 iterations; poor results were achieved with 1-50 iterations. The use of too many fixed variables also caused the LMA inversion to behave erratically, and so, using value ranges may be of greater importance than fixing parameters when using iterative optimization. However, it should be noted that fixed values were always used for the angular components of the PROSAIL model.

Figure 61 Measured and modelled TOC spectral-directional reflectance values for full spectrum ASD and simulated CHRIS/PROBA (ASD-M1) datasets for various field locations and all view zenith angles (VZA).

The greatest observed error between the measured and modelled directional spectra occurred in the lower wavelength regions (e.g. $< \sim 500$ nm) and generally occurred as an overprediction (i.e. modelled PROSAIL TOC reflectance values were greater than measured TOC reflectance values). Figure 62 shows the differences between the modelled and measured reflectance values for various sites and VZAs (modelled values were subtracted from measured values to better show over and

under prediction of PROSAIL). Reflectance at these wavelengths was either not well measured, as was discussed earlier with respect to inherent noise associated with spectroradiometers (Chapter 5), or not well modelled by the PROSAIL RTM. This was the case for both the ASD and M1 spectral datasets at all sites and VZAs. Similarly, more error was observed in the longer wavelength regions ($>\sim 900$ nm); however, in contrast to the shorter wavelength regions, these regions commonly produced underpredictions of TOC reflectance. Error patterns (both over and under predictions) were observed across the peak green reflectance (~ 550 nm), chlorophyll absorption (~ 680 nm), and red-edge regions (~ 700 - 750 nm) for all sites and VZAs. Although it could be stated that the degree of error for most spectral regions was well within 0.02, it is possible that these three regions are also not well modelled by PROSAIL in Arctic environments due to the complexity of the canopy (i.e. number of species, pigment pools) and the degree of spatial variation to canopy structure across all sites (i.e. gap fractions/soil contributions).

Finally, the high accuracy of the spectral matching (i.e. overall $\text{RMSE}=0.004 \pm 0.002$) may be attributable to the spatial averaging of subplots into plot scale measurements; more noise was observed in subplot spectra and this propagated through the inversion procedure.

Figure 62 Difference (Δ) between the modelled and measured TOC spectral-directional reflectance values for full spectrum ASD and simulated CHRIS/PROBA (ASD-M1) datasets for various field locations and all view zenith angles (VZA). Each plot shows all sampled spectra for the particular location and VZA (at the plot scale).

6.3.2. Inversion of the ASD and M1 datasets

The performance of the PROSAIL LMA inversion to estimate LCC, PAI_e , and CCC_e is shown in Table 34 below. Correlation coefficient (r^2) values are presented using a red/white/blue colour ramp to highlight poor (blue, $r^2=0$) to median (white, $r^2=0.5$) to optimal results (red, $r^2=1$). In total, 126 PROSAIL inversions were performed. Results are presented for all spectral datasets, vegetation variables, locations and angles. They vary significantly across the various datasets but the overall mean inversion results (r^2 and RMSE) were considered poor when compared against the empirical modelling retrievals (Chapter 5) using the exact same datasets and measurement scenarios (e.g., SR: $r^2=0.58$; ROSAVI: $r^2=0.54$; GPR: $r^2=0.62$). Inversion using the full ASD spectra achieved the best overall performance ($r^2=0.33$) compared to the M1 spectral subset ($r^2=0.28$).

Table 34 PROSAIL vegetation modelling inversion results for the field plot-scale datasets. Results are presented for both the ASD and M1 spectral datasets, and all view angles and field sites. Plotted relationships are bolded and marked with an asterisk.

Colour Scale (r^2)		ASD: Full Spectrum		CHRIS M1: Spectral Subset		
		Plot Scale		Plot Scale		
Location	VZA	Variable	r^2	RMSE	r^2	RMSE
Herschel Island (2011)	0°	LCC*	0.34	4.66	0.42	4.09
		PAI _e	0.18	0.38	0.10	0.35
		CCC _e	0.43	0.15	0.38	0.13
Banks Island (2012)	0°	LCC*	0.76	9.94	0.70	7.35
		PAI _e *	0.64	0.64	0.53	0.61
		CCC _e *	0.79	0.12	0.64	0.16
	-36°	LCC	0.68	8.91	0.66	7.16
		PAI _e	0.46	0.61	0.52	0.56
		CCC _e	0.70	0.12	0.60	0.16
	-55°	LCC	0.76	5.54	0.74	6.45
		PAI _e	0.51	0.48	0.25	0.50
		CCC _e	0.46	0.16	0.44	0.16
	+36°	LCC	0.64	7.82	0.65	7.52
		PAI _e	0.56	0.63	0.17	0.63
		CCC _e	0.67	0.17	0.49	0.20
	+55°	LCC	0.67	9.29	0.57	11.19
		PAI _e	0.46	0.52	0.13	0.56
		CCC _e	0.56	0.21	0.30	0.22
Richards Island (2013)	0°	LCC	0.31	8.15	0.15	9.28
		PAI _e	0.37	0.50	0.00	0.59
		CCC _e	0.37	0.24	0.01	0.25
	-36°	LCC*	0.33	8.05	0.52	5.20
		PAI _e	0.14	0.49	0.08	0.45
		CCC _e	0.11	0.23	0.19	0.19
	-55°	LCC	0.33	4.80	0.27	4.55
		PAI _e	0.05	0.39	0.07	0.49
		CCC _e	0.08	0.16	0.06	0.16
	+36°	LCC	0.17	9.98	0.11	6.91
		PAI _e	0.01	0.59	0.01	0.54
		CCC _e	0.07	0.27	0.05	0.23
	+55°	LCC	0.07	10.35	0.16	7.38
		PAI _e	0.04	0.44	0.31	0.39
		CCC _e *	0.59	0.20	0.13	0.18
Richardson Mountains (2013)	0°	LCC	0.47	4.51	0.28	6.51
		PAI _e *	0.25	0.26	0.44	0.17
		CCC _e	0.36	0.11	0.36	0.09
	-36°	LCC	0.03	11.97	0.03	11.90
		PAI _e	0.08	0.38	0.43	0.22
		CCC _e	0.02	0.22	0.16	0.14
	-55°	LCC	0.06	9.06	0.21	6.54
		PAI _e	0.12	0.40	0.21	0.27
		CCC _e	0.09	0.25	0.19	0.13
	+36°	LCC	0.09	10.56	0.12	8.55
		PAI _e	0.02	0.37	0.30	0.27
		CCC _e	0.19	0.16	0.42	0.11
	+55°	LCC	0.05	9.91	0.05	8.29
		PAI _e	0.39	0.32	0.25	0.29

		<i>CCC_e[*]</i>	0.27	0.16	0.22	0.14
<i>Richardson Mountains (2014)</i>	0°	<i>LCC</i>	0.40	8.91	0.15	7.60
		<i>PAI_e</i>	0.38	0.35	0.24	0.35
		<i>CCC_e</i>	0.48	0.15	0.30	0.15
	-36°	<i>LCC</i>	0.23	8.81	0.05	7.58
		<i>PAI_e</i>	0.12	0.46	0.11	0.38
		<i>CCC_e</i>	0.04	0.18	0.11	0.16
	-55°	<i>LCC</i>	0.26	9.00	0.01	12.03
		<i>PAI_e</i>	0.40	0.36	0.37	0.32
		<i>CCC_e[*]</i>	0.49	0.16	0.55	0.19
	+36°	<i>LCC</i>	0.10	8.37	0.08	9.56
		<i>PAI_e[*]</i>	0.28	0.34	0.53	0.30
		<i>CCC_e</i>	0.28	0.15	0.24	0.14
	+55°	<i>LCC[*]</i>	0.54	5.97	0.00	6.90
		<i>PAI_e[*]</i>	0.51	0.30	0.52	0.29
		<i>CCC_e</i>	0.50	0.14	0.24	0.15
<i>All sites</i>		<i>Overall</i>	0.33	-	0.28	-
	<i>All</i>	<i>LCC</i>	0.35	8.31	0.28	7.74
	<i>All</i>	<i>PAI_e</i>	0.28	0.44	0.27	0.41
	<i>All</i>	<i>CCC_e</i>	0.36	0.18	0.29	0.16
	0°	<i>LCC</i>	0.46	7.23	0.34	6.97
	-36°	<i>LCC</i>	0.32	9.44	0.32	7.96
	-55°	<i>LCC</i>	0.35	7.10	0.31	7.39
	+36°	<i>LCC</i>	0.25	9.18	0.24	8.14
	+55°	<i>LCC</i>	0.33	8.88	0.20	8.44
	0°	<i>PAI_e</i>	0.36	0.43	0.26	0.41
	-36°	<i>PAI_e</i>	0.20	0.49	0.29	0.40
	-55°	<i>PAI_e</i>	0.27	0.41	0.23	0.40
	+36°	<i>PAI_e</i>	0.22	0.48	0.25	0.44
	+55°	<i>PAI_e</i>	0.35	0.40	0.30	0.38
	0°	<i>CCC_e</i>	0.49	0.15	0.34	0.16
	-36°	<i>CCC_e</i>	0.22	0.19	0.27	0.16
	-55°	<i>CCC_e</i>	0.28	0.18	0.31	0.16
	+36°	<i>CCC_e</i>	0.30	0.19	0.30	0.17
	+55°	<i>CCC_e</i>	0.48	0.18	0.22	0.17
	0°	<i>All</i>	0.44	-	0.31	-
	-36°	<i>All</i>	0.25	-	0.29	-
	-55°	<i>All</i>	0.30	-	0.28	-
	+36°	<i>All</i>	0.26	-	0.26	-
	+55°	<i>All</i>	0.39	-	0.24	-

Visualization of the inversion results based on vegetation variable, spectral subset, geographic location, and VZA can be seen in Figure 63. Stratification by vegetation variable and spectral subset (i.e. the full spectrum dataset) with all VZAs combined produced higher mean r^2 values for CCC_e ($r^2=0.36$, RMSE=0.18) than for LCC ($r^2=0.35$, RMSE=8.31) or PAI_e ($r^2=0.28$, RMSE=0.44). A similar ranking was produced for the simulated M1 spectral subset but with

poorer results: CCC_e ($r^2=0.29$, $RMSE=0.16$), LCC ($r^2=0.28$, $RMSE=7.74$), and PAI_e ($r^2=0.27$, $RMSE=0.41$). The predicted relationships of LCC , PAI_e , and CCC_e are highly variable across each of the VZAs and appear almost random; i.e. the model is not generalizable across VZAs (Figure 63). Surprisingly, all $RMSE$ values were lower for the simulated M1 dataset than for the full spectrum ASD dataset (Table 34), despite the lower r^2 values for the M1 dataset.

Stratification of inversion results by location produced similar results to the empirical analysis. Banks Island (2012) produced the highest overall correlations for all vegetation variables (Figure 63, bottom right; LCC : $r^2=0.76$, $RMSE=9.94$; PAI_e : $r^2=0.64$, $RMSE=0.64$; CCC_e : $r^2=0.79$, $RMSE=0.12$). All other field sites produced much poorer relationships. The better correlation results for Banks Island may be due to the larger spatial variation observed for LCC , PAI_e , and CCC_e compared to the other field sites as discussed in detail in Chapter 5. However, it was surprising that the PROSAIL inversions had better correlations with LCC than PAI_e , since PAI_e generally showed better correlations/predictions with the empirical modelling approach (Chapter 5). Similar studies using PROSAIL have also reported that LAI is generally easier to predict/shows higher correlations than LCC (e.g. Darvishzadeh et al., 2008a).

Stratification of the inversion results by VZA also showed a high degree of variability (Figure 63, bottom left). The nadir VZA (0°) produced the best overall results ($r^2=0.44$), followed by $+55^\circ$ ($r^2=0.39$) for the full spectrum ASD dataset. Results for individual vegetation variables averaged over all sites showed the same pattern; optimal correlation results were achieved at 0° (LCC : $r^2=0.46$ $RMSE=7.23$; PAI_e : $r^2=0.36$ $RMSE=0.43$; CCC_e : $r^2=0.49$ $RMSE=0.15$) and $+55^\circ$ (LCC : $r^2=0.33$ $RMSE=8.88$; PAI_e : $r^2=0.35$ $RMSE=0.40$; CCC_e : $r^2=0.48$ $RMSE=0.18$). Scatterplots demonstrating these optimal PROSAIL inversions of the ASD dataset vs. measured field values

are shown in Figure 64 for various field sites and measurement scenarios. LCC relationships appear to show negative bias, whereas PAI_e and CCC_e show positive bias.

Figure 63 PROSAIL vegetation modelling correlation results. Clockwise from top left: (1) r^2 vs leaf/canopy variables, (2) r^2 of leaf canopy variables vs. view angle, (3) r^2 vs view angle, and (4) r^2 vs geographic location. Results are for both the ASD and M1 datasets. Boxplots show the interquartile range with factor of 1.5; outliers are displayed with a +.

Figure 64 Scatter plots for PROSAIL predictions/inversions for the three vegetation variables at various field locations using the ASD full spectrum dataset.

The M1 inversions; however, did not show the same strong results for 0° and +55°. Scatterplots demonstrating the optimal PROSAIL inversions of the simulated M1 dataset vs. measured field values are shown below (Figure 65) for various field sites and measurement scenarios (LCC, Herschel Island 0° and Richards Island -36°; PAI_e, Richardson Mountains 0° and Richardson Mountains +36°; CCC_e, Banks Island 0° and Richardson Mountains +36°). The same prediction biases can be observed in the M1 dataset as the ASD dataset; LCC relationships appear to show negative bias, whereas PAI_e and CCC_e show positive bias.

Figure 65 Scatter plots for PROSAIL predictions/inversions for various field locations using the M1 dataset.

6.3.3. Summary of prediction results

All combined plot scale modelling results based on NRMSE are presented in Table 35 below. NRMSE values are presented using a red/white/blue colour ramp to highlight poor (blue, NRMSE=0.50) to median (white, NRMSE=0.25) to optimal results (red, NRMSE=0.0). When all vegetation variables (LCC, PAI_e, and CCC_e) and VZAs were averaged across the field sites, it was shown that PROSAIL produced the best model accuracies for the M1 spectral subset (NRMSE=0.29) as compared to ASD full spectrum dataset (NRMSE=0.32). These results contrast with the r^2 results, where the ASD dataset produced the top correlations (mean r^2 =0.33) as compared to the M1 dataset (mean r^2 =0.28).

The vegetation variable that was best predicted across all sites was the CCC_e (mean value across all VZAs and datasets; NRMSE=0.24), followed by LCC (NRMSE=0.28) and PAI_e (NRMSE=0.40). Unlike the empirical predictions (Chapter 5), where mean prediction results (i.e. NRMSE) did not align with the r^2 results order (i.e. PAI_e produced the highest correlations but also produced the lowest accuracy), the accuracy of the PROSAIL inversions matched the results order

of the correlations (i.e. $CCC_e r^2=0.33$, $LCC r^2=0.32$, $PAI_e r^2=0.28$). The slightly better prediction of CCC_e as compared to LCC follows similar inversion based studies using PROSAIL (e.g. Darvishzadeh et al., 2008a); however, the relatively poor prediction of PAI_e in comparison to both CCC_e and LCC diverges from such studies (e.g. Curran et al., 1992; Baret & Jacquemoud et al., 1994). It is generally understood that there exists poor signal propagation from leaf to canopy scales (e.g. Asner et al., 1998; Jacquemoud et al., 1996); therefore, the estimates of PAI_e should show better results than the estimates of LCC. Finally, combined mean prediction results showed that all VZAs produced rather similar NRMSE values (e.g. mean values for all combined datasets $NRMSE=0.31\pm0.03$), with 0° producing the best overall mean predictions ($NRMSE=0.28$).

Table 35 NRMSE results for LMA inversions of PROSAIL. Results calculated across field sites have been combined.

<i>Colour Scale (NRMSE)</i>			<i>ASD: Full Spectrum</i>	<i>CHRIS M1: Spectral Subset</i>	<i>All</i>
			<i>LMA inversion of PROSAIL</i>	<i>LMA inversion of PROSAIL</i>	<i>All</i>
<i>Location</i>	<i>Angle</i>	<i>Variable</i>	<i>NRMSE</i>	<i>NRMSE</i>	<i>NRMSE</i>
<i>All</i>	<i>All</i>	<i>LCC</i>	0.28	0.27	0.28
	<i>All</i>	<i>PAI_e</i>	0.42	0.38	0.40
	<i>All</i>	<i>CCC_e</i>	0.25	0.23	0.24
	0°	<i>LCC</i>	0.25	0.23	0.24
	-36°	<i>LCC</i>	0.32	0.27	0.30
	-55°	<i>LCC</i>	0.26	0.28	0.27
	$+36^\circ$	<i>LCC</i>	0.31	0.29	0.30
	$+55^\circ$	<i>LCC</i>	0.29	0.28	0.29
	0°	<i>PAI_e</i>	0.41	0.40	0.40
	-36°	<i>PAI_e</i>	0.45	0.37	0.41
	-55°	<i>PAI_e</i>	0.38	0.37	0.38
	$+36^\circ$	<i>PAI_e</i>	0.46	0.41	0.43
	$+55^\circ$	<i>PAI_e</i>	0.37	0.36	0.37
	0°	<i>CCC_e</i>	0.21	0.21	0.21
	-36°	<i>CCC_e</i>	0.26	0.23	0.24
	-55°	<i>CCC_e</i>	0.26	0.23	0.24
	$+36^\circ$	<i>CCC_e</i>	0.26	0.24	0.25
	$+55^\circ$	<i>CCC_e</i>	0.25	0.24	0.25
	0°	<i>All</i>	0.29	0.28	0.28
	-36°	<i>All</i>	0.35	0.29	0.32
	-55°	<i>All</i>	0.30	0.29	0.30
	$+36^\circ$	<i>All</i>	0.34	0.31	0.33
	$+55^\circ$	<i>All</i>	0.30	0.30	0.30
<i>All</i>	<i>All</i>	<i>All</i>	0.32	0.29	-

6.3.4. Predicted model variables (leaf and canopy)

Summary statistics (mean, mode, standard deviation) calculated from the inverted/predicted PROSAIL parameters from both spectral subsets are shown in Table 36. The PROSAIL model parameters not measured in the field were as follows: the leaf structure parameter (N), the leaf brown pigment content (C_{bp}), canopy hotspot size (S_L), soil brightness parameter (P_S), and the fraction of diffuse incoming solar radiation ($SKYL$). The only surprising result from the inversions is the $SKYL$ values, which are substantially higher than values encountered/used in other studies with similar vegetation types (e.g. Darvishzadeh et al., 2008a; Verrelst et al., 2015a). It is likely that these values are higher because of the generally low SZAs encountered in the Arctic as opposed to SZAs encountered at mid-latitude and tropical sites; most incoming/incident solar radiation in the Arctic may be received as diffuse sky radiation. Other reasons for high $SKYL$ values may be due to the many spectral measurements taken on cloudy days.

All PROSAIL parameters obtained at the field scale were later used to inform the inversion of satellite CHRIS/PROBA spectra (i.e. starting values and value ranges) as described in Chapter 7. The combined parameter averages and value ranges of the inversions for all sites and VZAs were used to generalize the approach across the bioclimatic gradient (i.e. sites) with parameterization values that could be considered more appropriate for Arctic conditions (discussed further in Chapter 7).

Table 36 Statistics for modelled values from the PROSAIL inversion. Values were used to further constrain the inversion at the remote sensing scale. Values indicated with an asterisk are based on fixed values for each inversion (known values for each plot).

<i>Model</i>	<i>Symbol</i>	<i>Units</i>	<i>Mean Modelled Values (ASD)</i>	<i>Mode (ASD)</i>	<i>Standard deviation (SD)</i>	<i>Mean Modelled Values (M1)</i>	<i>Mode (M1)</i>	<i>Standard deviation (M1)</i>
PROSPECT-5	<i>N</i>	Unitless	1.61	2.50	0.54	1.35	2.50	0.64
	<i>C_{ab} (LCC)</i>	µg/cm ⁻²	33.99	0.00	12.91	34.28	0.00	11.88
	<i>C_{ar}</i>	µg/cm ⁻²	16.02	25.00	6.85	17.19	25.00	6.51
	<i>C_{bp}</i>	Unitless	0.50	0.00	0.41	0.43	0.00	0.34
	<i>C_w</i>	g/cm ⁻²	0.03	0.00	0.01	0.02	0.00	0.02
	<i>C_m</i>	g/cm ⁻²	0.04	0.03	0.04	0.04	0.00	0.04
SAILH	<i>LAI (PAI_e)</i>	m ² m ⁻²	1.26	1.10	0.35	1.19	1.06	0.32
	<i>ALA</i>	Deg	48.49	35.00	6.35	45.44	35.00	6.48
	<i>S_L</i>	m m ⁻¹	0.09	0.10	0.02	0.06	0.10	0.04
	<i>P_s</i>	Unitless	1.11	1.50	0.42	1.10	1.50	0.40
	<i>SKYL</i>	Unitless	57.26	0.01	18.75	57.02	100.00	25.45
	<i>SZA*</i>	Deg	-	-	-	-	-	-
	<i>VZA*</i>	Deg	-	-	-	-	-	-
	<i>RAA*</i>	Deg	-	-	-	-	-	-

6.4. Discussion and Conclusions

A field-based, multi-angle spectroscopic analysis of Arctic vegetation was conducted across a bioclimatic gradient in the Western Canadian Arctic using a one-dimensional turbid medium radiative transfer model and a numerical optimization based inversion methodology. The results showed that the PROSAIL model was not capable of accurately/reliably simulating radiation transfer in heterogeneous Arctic tundra canopies across a diversity of landscapes and across various sun-target-sensor geometries when inverted using the Levenberg-Marquardt numerical optimization algorithm (mean of all inversions: $r^2=0.31$, NRMSE=0.30). Key findings of these assessments are presented here in regard to the following: (1) assessment of the predicted vegetation variables (LCC, PAI_e, or CCC_e), (2) the applicability of using PROSAIL in Arctic environments (i.e. the use of a one-dimensional turbid medium model in a heterogeneous

assemblage) and its generalizability across the various measurement scenarios (i.e. model generalizability across stratified measurement scenarios); (3) the applicability of LMA inversion and possible ways forward with regularization methods (e.g. inversion starting values, fixed variables, and the use of spectral subsets); and (4) the overall conclusion and questions applied to the physical studies of Chapter 7.

(1) The effective canopy chlorophyll content (CCC_e) is a synthetic parameter/variable (i.e. $LCC \times PAI_e$). Its inclusion in the analysis allowed for the assessment of whether canopy reflectance was a better predictor of leaf or canopy chlorophyll content (Darvishzadeh et al., 2008a). In most scenarios, the inversion of PROSAIL produced stronger relationships (r^2) and predictions (NRMSE) with CCC_e than LCC or PAI_e . This outcome may be attributable to the information content that exists within the variable itself; LCC and PAI_e are known to conjointly control canopy reflectance (Darvishzadeh et al., 2008a; Stagakis et al., 2010; Ollinger, 2011; Verrelst et al., 2016) and thus combining these two variables into one product (a) produces a synergistic vegetation parameter/variable (representative of both variables) and (b) reduces variance with the effect of improving modelled results. Further, this result (i.e. the enhanced retrieval of CCC_e) agrees with the empirical modelling results (Chapter 5) and with similar PROSAIL-based retrieval studies (e.g. Darvishzadeh et al., 2008a). In most measurement scenarios (e.g. VZAs, field sites), PROSAIL produced better estimates of LCC than PAI_e (NRMSE=0.40 and NRMSE=0.28, respectively). This result aligns with the empirical retrievals (Chapter 5) that produced overall superior estimates for LCC as opposed to PAI_e (NRMSE=0.15 and NRMSE=0.21, respectively). Regarding the physically-based retrievals of PAI_e , it is possible that the PROSAIL model is not adequately simulating reflectance in the red-edge and the left wing of the NIR wavelength regions (greatest error centered at approximately 700 nm), which are regions known to be sensitive to canopy and

leaf structure in Arctic vegetation canopies (as was shown in the modelled-measured relative error analysis, Figure 62) (Buchhorn et al., 2013; Liu et al., 2017). However, the modelled spectra were very close in agreement with the measured spectra within all spectral regions (reflectance error differences of $\sim\pm 0.02$). It is also possible that TOC reflectance is not being accurately modelled with respect to sun-target-sensor geometry since the results, when stratified per VZA, are quite variable. Although LCC produced superior results to PAI_e, it should be stated that the relationships between measured and estimated LCC were poor in all inversion scenarios when averaged across the bioclimatic gradient. These results align with studies that have shown difficulties in estimating leaf chlorophyll content with PROSAIL in heterogeneous plant assemblages (Curran et al., 1992; Baret & Jacquemoud, 1994; Darvishzadeh et al., 2008a), but differ from studies that show leaf area is easier to predict than leaf chlorophyll content (Darvishzadeh et al., 2008a; Atzberger et al., 2015). As previously stated, these studies typically point towards poor signal propagation from leaf to canopy (Asner, 1998; Jacquemoud et al., 1996; Yoder & Pettigrew-Crosby, 1995). Thus, canopy variables should always be easier to estimate than leaf based variables.

(2) The overall poor results of the inversions may be explained by the inability of the one-dimension PROSAIL turbid medium model to accurately describe the radiation field of a complex three-dimensional heterogeneous canopy (e.g., gap fractions, clumping effects, multiple leaf layers having different optical characteristics, etc.). If the assumptions of the turbid medium are violated, it is expected that the PROSAIL model will not be able to realistically simulate TOC reflectance, and therefore the retrieved biochemical and biophysical variables can be expected to be biased, ambiguous, or simply wrong (Meroni et al., 2004; Darvishzadeh et al., 2008a). Improvement in parameter/variable retrieval may be expected from models that explicitly consider canopy heterogeneities such as clumping effects, varying leaf structures, and pigment variability as it

relates to species present (e.g. Verhoef & Bach, 2007; Feret et al., 2017); however, spatial and species-based heterogeneity can be considered scale dependent and tricky to handle effectively in a modelling scenario (Darvishzadeh et al., 2008a). For example, it is difficult to determine the point at which scale is no longer a factor, or to determine the scale at which the canopy begins to act more as a single turbid medium and is less under the influence of its individual absorbing and scattering components. Although the inversion of the subplot spectral measurements was not fully investigated, the use of averaged conditions across the subplot scale was believed to have resolved the effects of noise and spatial heterogeneity at the plant and subplot scales ($< 1 \text{ m}^2$). Darvishzadeh et al. (2008a) showed that low-level, heterogeneous grassland canopies can be simulated with the PROSAIL one-dimensional turbid medium model; however, the results of their study demonstrated that the stratification of plant heterogeneity (based on the number of species present) must be conducted to increase accuracy, further suggesting that PROSAIL is not well suited to naturally complex and heterogeneous multi-species canopies such as Arctic tundra. A similar approach using the stratification of Arctic tundra based on species numbers would be a difficult undertaking due to the natural mixture of species at the subplot scale (1 m^2), and would therefore not be practical to implement within an ecosystem monitoring program. Nevertheless, the use of PROSAIL may be of value to monitoring monotypic shrub patches as their abundance increases across the Arctic (Sturm et al., 2001; Fraser et al., 2014a) and as high spatial and spectral resolution sensors become more available.

In this study, the Banks Island field site showed the best average correlations compared to the other field sites, but showed high error. This demonstrates the importance of sampling across multiple geographic locations within an ecosystem to fully assess the generalizability of the physical model approach. It is common for studies to not include a geographically diverse field

sample when testing the full functionality/generalizability of a model (i.e. testing its physical assumptions) as it would be implemented within a monitoring program. The simple reason is that multi-location field work is often expensive and logistically difficult to implement, particularly in remote areas; in this study four field campaigns in separate years were required to acquire all the field data. Additionally, this study tested the directional capabilities of the PROSAIL model; it produced the best correlation results at 0° and $+55^\circ$ compared to the empirical analysis (Chapter 5) which showed optimal correlation performance at -55° . The differences in results across the view angles establishes two possible uncertainties: (i) the model is not fully capable of accounting for directional reflectance (or possible problems with model parameterization) and (ii) the inversion approach is not accounting for the ill-posed problems associated with RTMs (i.e. multiple solutions may exist to the model inversion). It is also possible that the model is not being parameterized correctly, but this is the least unlikely factor.

(3) The LMA iterative numerical optimization inversion technique has not been extensively tested with the PROSAIL RTM (e.g. Hilker et al., 2017) and has never been tested in Arctic tundra ecosystems to retrieve vegetation biochemical and biophysical parameters/variables from TOC multi-angle spectral reflectance. In this study, it was shown that the algorithm is capable of iterating the PROSAIL leaf and canopy parameter space to accurately simulate Arctic tundra TOC spectral reflectance across multiple field sites and varying sun-target-sensor geometries; however, the overall results of the parameter/variable inversions were poor. Considerations regarding the implementation of the LMA inversion strategy as learned in this study are as follows.

(i) Iterative optimization is a slow computational process and does not present itself (with current single workstation computing speeds) as a feasible solution for extensive mapping and monitoring; however, iterative optimization can be considered a useful tool for determining the

parameter space of unknown variables as it provides a straightforward means for testing model and parameter effectiveness. To fully evaluate the robustness of the PROSAIL model in Arctic environments, LMA inversion should be tested against other accepted retrieval algorithms, such as LUTs and ANNs since they have been shown to produce acceptable results and can be implemented into large scale mapping and monitoring initiatives (Darvishzadeh et al., 2008a; Atzberger et al., 2015; Verrelst et al., 2015b; Rivera et al., 2013). However, this may be of no consequence since iterative numerical optimization is also capable of accurate inversion results (Hilker et al., 2017; Feret et al., 2017). Lastly, comparative inversion methods studies are nonexistent for Arctic environments.

(ii) The LMA inversion as implemented in this study allows for regularization strategies, such as setting upper and lower parameter bounds, as well as fixing function parameters. Field-based measurements and known sun-target-sensor geometries were used to constrain the inversion space/model parameters in this study, Regularization is a common and efficient approach to circumventing ill-posedness of the inversion while improving the accuracy of the estimated canopy variables (Combal et al. 2003; Meroni et al. 2004; Rivera et al., 2013). An interesting outcome of the inversion results was that all fourteen leaf and canopy parameters reached their upper and lower boundaries on multiple occasions (for both the full spectrum and simulated M1 datasets). It is possible that either some wavelengths were poorly measured (i.e. too much noise/instrument error) or the model could not adequately simulate the TOC spectral reflectance by means of the chosen parameter space. However, as Darvishzadeh et al. (2008a) showed, the expansion of the parameter space (e.g. upper and lower boundaries of the parameters) does not necessarily lead to amelioration of results and, in the case of numerical optimization, greatly increases the inversion time. Experimentation in this study also showed that fixing too many parameters caused the LMA

algorithm to fail outright (due to local minima being encountered), even when those parameters were measured and represented the actual conditions represented in the model. It is possible that further limiting the parameter space, but not fixing parameters, may provide the best regularization approach for numerical optimization. It may also be possible to produce a LUT using various iteration values (e.g. 100, 1000, 2500, 5000) within the defined parameter space and taking the mean of the solutions.

(iii) A spectral subset, consistent with the CHRIS/PROBA M1 band set, was tested in the LMA inversion procedure. It was shown that the use of less spectral information led to overall poorer correlation results than the full spectrum ASD dataset; however, the M1 spectral subset produced lower overall error. The better correlations achieved with the full spectrum dataset are similar to results achieved by Darvishzadeh et al. (2008a), who demonstrated that the use of less spectral information can lead to inferior results; however, in their study only a few carefully chosen bands were used. Nevertheless, it has been demonstrated in other studies (Meroni et al., 2004; Schlerf & Atzberger, 2006) that the selection of a few wavebands will often give better results than those achieved using the full spectral resolution.

(iv) Finally, although not explored in this study, the choice of merit/cost function can also play a role in the inversion accuracy, albeit not a large role, and could be explored in future studies using iterative optimization (Rivera et al., 2013). The merit function used in this study (Pearson chi-square) has been tested against other divergences (see Rivera et al., 2013).

(4) The overall conclusion drawn from this study was that the PROSAIL model when inverted using the LMA was determined to be ill-suited for the prediction of LCC, PAI_e, and CCC_e in Arctic tundra environments using field-based spectral data. Chapter 7 extends this analysis to the remote sensing scale.

Chapter 7. Retrieval of Arctic Vegetation Biophysical and Biochemical Properties from CHRIS/PROBA Multi-Angle Imaging Spectroscopy using Empirical and Physical Modelling

Abstract

In this study, three previously investigated modelling approaches were used to predict leaf chlorophyll content (LCC , $\mu\text{g}/\text{cm}^2$), effective plant area index (PAI_e , m^2/m^2), and effective canopy chlorophyll content ($[CCC_e = LCC \times PAI_e]$, g/m^2) across a bioclimatic gradient in the Western Canadian Arctic using multi-angle CHRIS/PROBA Mode-1 (M1) spectroscopic satellite data. Modelling approaches included: (1) parametric linear regression based on robust multi-band and predefined narrowband vegetation indices (VIs), (2) non-parametric machine learning Gaussian Processes Regression (GPR), and (3) the inversion of the PROSAIL radiative transfer model using the Levenberg-Marquardt algorithm (LMA) iterative numerical optimization. Modelling results obtained from the previous ground-based empirical and physical investigations were used to inform the modelling approach used here. Multi-angle CHRIS/PROBA M1 imagery (-55° , -36° , 0° , $+36^\circ$, $+55^\circ$) was acquired over four field sites situated across the Yukon and Northwest Territories, Canada between the years 2011 to 2014. Efforts were made to collect biochemical and biophysical field measurements concomitant with satellite image acquisitions. Multi-angle spectra extracted from the CHRIS/PROBA imagery were processed using all three modelling methods and compared against field measurements. The results of the empirical analysis (i.e. VIs and GPR) showed that the best overall modelling results based on r^2_{cv} (cv = cross validated) were achieved with the GPR approach at the plot scale (mean $r^2_{cv}=0.59$, across all VZAs), followed by the multi-band simple ratio (SR) VI (mean $r^2_{cv}=0.53$, across all VZAs) and lastly the revised optimized soil adjusted vegetation index (ROSAVI) (mean $r^2_{cv}=0.48$, across all VZAs). However, best predictive

performance was achieved by SR (mean $\text{NRMSE}_{\text{cv}}=0.14$; NRMSE = normalized RMSE) followed by GPR (mean $\text{NRMSE}_{\text{cv}}=0.16$) and ROSAVI (mean $\text{NRMSE}_{\text{cv}}=0.17$). The results of the physically-based PROSAIL inversion demonstrate that the investigated vegetation variables (LCC , PAI_e , and CCC_e) cannot be estimated through the inversion of a radiative transfer model with accuracies comparable to those of empirical approaches. Furthermore, regularization strategies applied to the LMA inversion did not ameliorate prediction results. Inversion of the PROSAIL model yielded a (non-cross-validated) correlation of $r^2=0.28$ and accuracy $\text{NRMSE}=0.27$ irrespective of view zenith angle (VZA) and geographic location (i.e., when all results were combined). This ranking of modelling method performance is the same as was found in the field studies of Chapters 5 and 6 (e.g. GPR mean $r^2_{\text{cv}}=0.61$, $\text{NRMSE}_{\text{cv}}=0.16$; SR $r^2_{\text{cv}}=0.51$, $\text{NRMSE}_{\text{cv}}=0.15$; ROSAVI $r^2_{\text{cv}}=0.45$, $\text{NRMSE}_{\text{cv}}=0.18$; PROSAIL mean $r^2=0.33$, $\text{NRMSE}=0.32$). The overall best performing VZA for both empirical and physical modelling approaches was $+55^\circ$ (mean $r^2=0.45$ of all methods combined, $\text{NRMSE}=0.19$), while surprisingly nadir (0°) VZAs produced the worst model fits (mean $r^2=0.33$, $\text{NRMSE}=0.18$). Overall, prediction accuracies for all view angles were very similar (mean of all methods combined, $\text{NRMSE}_{\text{cv}}=0.18\pm0.01$), indicating no distinct advantage for any one VZA. This leads to the conclusion that multi-angle imaging spectroscopy provides no added benefit over fixed-angle remote sensing platforms for chlorophyll or plant area index estimation in Arctic environments using the methods analyzed in this study. The field-based multi-angle prediction results showed almost identical results (for all methods combined at the plot scale, mean $\text{NRMSE}_{\text{cv}}=0.19\pm0.01$), further indicating that field sampling was conducted at an appropriate spatial scale. Finally, this study emphasizes the need for testing biochemical and biophysical variable extraction methodologies across field sites within the context of a larger ecosystem.

7.1. Introduction

In the previous field-scale studies of this thesis (Chapters 5 and 6), three modelling approaches were evaluated for predicting leaf chlorophyll content (LCC, $\mu\text{g}/\text{cm}^2$), effective plant area index (PAI_e , m^2/m^2), and effective canopy chlorophyll content ($[\text{CCC}_e = \text{LCC} \times \text{PAI}_e]$, g/m^2) across a bioclimatic gradient in the Western Canadian Arctic. The methods used for estimating vegetation variables from the imaging spectrometer data comprised of two distinct approaches: empirically-based modelling (e.g. Verrelst et al., 2015a,b) and physically-based modelling (e.g. Jacquemoud et al., 2009). A review of both modelling methodologies has been provided previously (Chapters 2, 5, and 6). The three modelling approaches used in these studies included: (1) parametric linear regression based on multi-band and predefined narrowband vegetation indices (VIs), (2) non-parametric machine learning Gaussian Processes Regression (GPR), and (3) the inversion of the PROSAIL radiative transfer model (RTM) using the Levenberg-Marquardt algorithm (LMA) iterative numerical optimization. The modelling results obtained from the previous field-based empirical and physical investigations were used to inform the modelling approach used at the remote sensing scale, and include the following implementation strategies. (1) The simple ratio (SR) and revised optimized soil adjusted vegetation index (ROSAVI) were determined to be the optimal multi-band and predefined multi-angle VIs, respectively. All remote sensing data were processed with these VIs. The optimal multi-angle spectral regions for variable retrievals (LCC, PAI_e , and CCC_e) were shown to be largely within 450-550 nm and 650-750 nm; however, due to the large degree variable covariation observed in the band selections across view zenith angles (VZAs), the remote sensing analyses were conducted with the full spectral dimensionality of the sensor. (2) At the field-scale, the GPR algorithm produced favorable results when used in combination with a spectrally reduced dataset (i.e. one that was analogous to the sensor used in

this study). Consequently, the full spectral dimensionality of the remote sensing data used in this study was deemed appropriate (i.e. optimal) for use with GPR; accordingly, the GPR algorithm was programmed to remove one band for each model iteration. (3) The inversion of PROSAIL using the LMA was shown to produce inaccurate results at the field-scale; however, its implementation at the remote sensing scale was completed to investigate: (a) prediction accuracy across spatial scales (i.e. are the assumptions and modelling results maintained between the field and remote sensing scales?); and (b) regularization strategies (i.e. can further regularization of the original parameter space improve inversion results?).

The previous literature reviews of this thesis (Chapters 2, 5, and 6) have shown the following. (1) Arctic vegetation-based spectroscopic remote sensing investigations have only been conducted at the field-scale and not from satellite platforms (e.g. Liu et al., 2017; Bratsch et al., 2016; Buchhorn et al., 2013; Davidson et al., 2016; Hope et al., 1993; Huemmrich et al., 2013; Kushida et al., 2009, 2015; Laidler et al., 2008; Riedel et al., 2005a,b; Ulrich et al., 2009). (2) There are currently no studies that have measured foliar biochemical quantities in the field (e.g. LCC or CCC_e) for remote sensing retrieval purposes. (3) There have not been any satellite-based imaging spectroscopy studies in the Arctic that have compared empirical and physical retrieval methods for modelling biophysical or biochemical variables from tundra vegetation. Specifically, no studies have compared the retrieval capabilities of narrowband VIs, GPR, and the inversion of PROSAIL for estimation of LCC, PAI_e, and CCC_e in the Western Canadian Arctic. (4) Arctic remote sensing studies have shown that the optical properties of Arctic biomass are complicated by numerous factors (see Chapter 5), including illumination conditions and sensor viewing geometry (e.g. view zenith angles, VZAs) (Asner, 1998; Curran, 1989; Stow et al., 2004; Feret et al., 2008; Juszak et al., 2014; Liu et al., 2017). This point is of interest since no studies have examined the extraction

of Arctic biophysical and biochemical variables from multi-angle spectroscopic instruments, let alone comparing the above mentioned empirical and physical extraction methods using multi-angle spectroscopic data. The multi-angle approach was realized using the Compact High Resolution Imaging Spectrometer (CHRIS) sensor onboard the Project for On-Board Autonomy (PROBA) platform (CHRIS/PROBA) (Barnsley et al., 2004). Imaging spectroscopy and multi-angle remote sensing have been reviewed previously (Chapters 2 and 5).

In consideration of the above, the objective of this study was to estimate LCC, PAI_e and CCC_e in Arctic tundra environments across a latitudinal gradient using the above described empirical and physical modelling approaches in combination with multi-angle CHRIS/PROBA full spatial and spectral resolution data (Mode-1, M1). The suitability of the methods is analyzed in terms of the strength of the model fit and the prediction accuracy for estimating of LCC, PAI_e, and CCC_e (e.g. the coefficient of determination, r^2 ; the root mean square error, RMSE; and the normalized RMSE, NRMSE, respectively).

7.2. Materials and Methods

7.2.1. Study sites

The study areas of the remote sensing analysis were based on the field locations detailed earlier in the thesis (Chapter 2). Field sites used for the remote sensing analysis included Herschel Island, YT (centre of the nadir CHRIS/PROBA acquisition, 69.58° N, -139.05° W), Banks Island, NT (74.19° N, -120.64° W), and the Richardson Mountains, YT, NT (67.05° N, -136.21° W). Due to the poor image quality (e.g. cloud contamination, noise), lack of image acquisitions, or too great of a gap between fieldwork and image acquisition dates, the Tuktoyaktuk, NT (2012) and Richards Island, NT (2012 and 2013) field sites were excluded from the analysis. The selection of field sites and image acquisitions represents a bioclimatic gradient extending from 67° N to 75° N across the

Western Canadian Arctic. All field sites were visited and sampled between July 10th and August 4th in given years between 2011 and 2014 during what is considered the peak of the growing seasons to minimize any phenological variability introduced by the short tundra growing season. Table 23 (Chapter 5, Section 5.2.2.) shows the date and time range that each location was sampled on the ground.

7.2.2. Ground data and spectral measurements

Field-sample design and the measurements of leaf chlorophyll content (LCC, $\mu\text{g}/\text{cm}^2$), leaf area index (previously described as effective plant area index, PAI_e , m^2/m^2 , and used as such hereafter), canopy chlorophyll content (effective canopy chlorophyll content, CCC_e , g/m^2 , hereafter), and multi-angle field spectra were completed at each site and are described previously in Chapter 5. An in-depth description of the LCC sampling and processing can be found in Chapter 3. The description of the measurement and modelling of PAI_e can be found in Chapter 4. Description of the field-based multi-angle spectral sampling can be found in Chapter 5. Destructive measurements of foliar and canopy carotenoid content, equivalent water thickness (EWT), and dry matter content (leaf mass) acquired in the Richardson Mountains during the 2014 field season (as described in detail in Chapter 4) were used as accepted modelling values across all sites, as dominant vegetation types remained (to a certain extent) consistent across sites. Where applicable, destructive measurements were used to parametrize the physical modelling approach. All biochemical and biophysical variables hereafter assume the measurement systems above.

Field scale plots and subplots were established as described in previous chapters (see Chapters 4, 5 and 6). The total number of plots (109) were divided as follows: (1) Herschel Island (2011) 33 plots, (2) Banks Island (2012) 31 plots, (3) Richardson Mountains (2013) 25 plots, (4) Richardson Mountains (2014) 20 plots. Because the footprint of the CHRIS/PROBA sensor is

different for each acquisition look angle, on the ground sample sizes differ per CHRIS/PROBA view zenith angle (VZA). In some instances, ground plots were not useable as they were outside of the instantaneous field of view (IFOV) of the sensor. The following sample sizes were obtained for each VZA at each field site (-55° , -36° , 0° , $+36^{\circ}$, $+55^{\circ}$, respectively): Herschel Island (2011) $n=25, 33, 25, 33, 25$; Banks Island (2012) $n=25, 27, 31, 31, 27$; Richardson Mountains (2013) $n=19, 21, 25, 23, 19$; Richardson Mountains (2014) $n=11, 19, 20, 20, 14$.

7.2.3. Satellite image acquisitions

Multi-angle CHRIS/PROBA M1 imagery was acquired over Herschel Island (2011), Banks Island (2012), and Richardson Mountains (2013 and 2014). The CHRIS/PROBA sensor specifications have been described in Chapters 2 and 5. Table 37 shows the acquisition dates and times and the associated sun-target-sensor geometry for each image. Due to the poor quality of the CHRIS/PROBA metadata products associated with some of the images, steps were taken to correct errors. For example, the acquisition dates and times of the Richardson Mountains 2014 imagery were deemed to be completely incorrect when compared against previous overpass times occurring at a similar time of year (and using the sun angles and position of shadows in the image). Dates and times were therefore estimated. Additional problems encountered with metadata included missing or erroneous values for sun and sensor positions. Sun positions were updated using the Sun Earth Tools (<https://www.sunearthtools.com>) using estimated overpass times. VZA and VAA, where missing or deemed incorrect, were estimated using a 1st order derivation based on a tool created by White and Alonso (2016). Corrected time and angle values are shown in Table 37 (bolded). Figure 66 shows the uncorrected image acquisitions that were used in the study. All images are shown as colour composites using bands 23 (red, 651 nm), 13 (green, 551 nm), and 3 (blue, 452 nm). Details worth mentioning include: (1) sparse vegetation in the Banks Island

acquisitions appears extremely dark as compared to the other field sites due to the sparse vegetation, and (2) theoretical and actual VZAs differ for each CHRIS/PROBA product (see Table 37). Finally, working with CHRIS/PROBA was extremely time consuming and frustrating due to missing metadata, flipped/mirrored raw images, and processing errors encountered with the proprietary processing software (BEAM VISAT).

Table 37 CHRIS/PROBA image products with associated acquisition and sun angles. Bolded values were updated (estimated) or corrected from the metadata delivered with the images (see text). Acronyms are: view zenith angle (VZA), view azimuth angle (VAA), sun zenith angle (SZA), sun azimuth angle (SAA), and relative azimuth angle (RAA; the angular azimuth difference between the sun and sensor). It should be noted that the theoretical VZA and actual VZA differ.

<i>Image Location</i>	<i>Acquisition Date</i>	<i>Time</i>	<i>VZA</i>	<i>VZA (Actual)</i>	<i>VAA</i>	<i>SZA</i>	<i>SAA</i>	<i>RAA</i>
<i>Herschel Island, NT</i>	<i>July 20, 2011</i>	18:38:33	0°	15.12	138.46	66.90	267.03	128.57
		18:37:44	+36°	32.22	35.14	66.81	266.79	128.35
		18:39:23	-36°	34.94	176.77	66.99	267.26	90.49
		18:36:55	+55°	51.82	27.89	66.73	266.56	121.33
		18:40:12	-55°	53.23	187.49	67.07	267.50	80.01
<i>Banks Island, NT</i>	<i>August 1, 2012</i>	17:27:05	0°	9.00	300.05	66.18	250.10	49.95
		17:26:16	+36°	36.69	12.53	66.12	249.85	122.68
		17:27:54	-36°	36.69	222.57	66.18	250.10	27.53
		17:25:27	+55°	55.22	18.28	66.05	249.59	128.69
		17:28:44	-55°	55.22	216.83	66.24	250.35	33.52
<i>Richardson Mountains, YT/NT</i>	<i>August 2, 2013</i>	16:19:43	0°	21.00	137.52	57.94	235.36	97.84
		16:18:00	+36°	39.67	48.62	57.86	235.09	173.53
		16:20:32	-36°	38.20	167.46	58.02	235.62	68.16
		16:18:06	+55°	53.65	28.82	57.86	235.09	153.73
		16:21:21	-55°	55.29	180.44	58.14	235.88	55.44
<i>Richardson Mountains, YT/NT</i>	<i>July 6, 2014</i>	17:02:00	0°	20.05	290.48	56.81	248.83	41.65
		17:01:00	+36°	39.36	353.48	56.81	248.62	104.86
		17:03:00	-36°	39.36	227.49	56.81	249.03	21.54
		17:00:00	+55°	56.12	0.21	56.81	248.41	111.80
		17:04:00	-55°	56.12	215.75	56.81	249.24	33.49

<i>VZA</i>	<i>Herschel Island (2011)</i>	<i>Banks Island (2012)</i>	<i>Richardson Mountains (2013)</i>	<i>Richardson Mountains (2014)</i>
0°
$+36^{\circ}$
-36°
$+55^{\circ}$
-55°

Figure 66 Uncorrected multi-angle CHRIS/PROBA M1 images acquired over the various field sites. All acquisition angles (VZAs) are shown. All images are shown as colour composites using bands 23 (red, 651 nm), 13 (green, 551 nm), and 3 (blue, 452 nm).

Polar plots showing the sun and sensor acquisition geometry of the above images can be seen in Figure 67. The polar plots demonstrate which view angles capture either forward or backscattering radiation. Generally, all forward looking (i.e. positive look angles) capture forward scattering radiation, and negative look angles capture backscattering radiation.

Figure 67 Polar plots showing the sun and sensor (CHRIS/PROBA) positions relative to acquisition scene center.

7.2.4. Satellite image preprocessing

Prior to spectral extraction and modelling, CHRIS/PROBA imagery was preprocessed using the CHRIS/PROBA Toolbox software developed as an extension for the VISAT BEAM version 5.0 (Brockmann Consult, <https://www.brockmann-consult.de/beam>). Preprocessing of all images (as expressed in Figure 68) consisted of: (1) de-stripping and noise reduction of raw imagery, (2) cloud masking, (3) atmospheric correction and generation of columnar water vapour map, and (4) geometric correction and orthorectification. Because of the inability of the VISAT BEAM tool to produce accurate georeferenced products, images were orthorectified using Geomatica's OrthoEngine (PCI Geomatics, 2016) and Toutin's rigorous model (Toutin et al., 1992; Toutin, 2004; Poli & Toutin, 2012; Belfiore & Parente, 2016).

Figure 68 Processing chain for CHRIS/PROBA imagery are as follows (from top left): raw imagery, noise reduction, probabilistic cloud masking, atmospheric correction, columnar water vapour generation, and geometric correction and orthorectification.

Noise reduction: All CHRIS/PROBA imagery is affected by two types of noise. The first can be defined as random noise, which varies with time and determines the minimum signal-to-noise ratio of the sensor (Aiazzi et al., 2002; Wettle et al., 2004; Gómez-Chova et al., 2008a,b). The second is coherent noise characterized by non-periodic deterministic disturbance patterns that develop during image formation; these patterns are characterized by spatial and spectral coherence and are a known problem (Barducci & Pippi, 2001; Barducci et al., 2005; Gómez-Chova et al., 2008a). For example, transmissions of channel 2 randomly produce anomalous drop-outs in image rows (Gómez-Chova et al., 2008a,b). These types of gaps can be filled in by interpolating from values of neighbouring pixels and spectral bands (Gómez-Chova et al., 2008a,b). The CHRIS sensor is also affected by vertical striping in the image columns (as evident in Figure 68, top left) due to irregularities in the entrance slit and sensor elements (Gómez-Chova et al., 2008a,b). Although gain correction factors have been applied to the sensor, these patterns are known to be dependent on sensor temperature and must be corrected prior to data use (Gómez-Chova et al., 2008a). All CHRIS/PROBA images obtained for this research were therefore corrected for these types of noise using the algorithm of Gómez-Chova et al. (2008a) as it is implemented within the CHRIS/PROBA Toolbox. The noise reduction algorithm was parameterized to apply the slit correction using a smoothing order of 27 pixels. Drop-out correction was applied using five neighbouring bands and a 4-connected neighbourhood type.

Cloud masking: The accurate and automatic detection of clouds in satellite scenes is an important issue for a wide variety of remote sensing applications. Clouds are a significant error source in biochemical and biophysical variable retrieval (Gómez-Chova et al., 2008c), especially in the Arctic where cloud contamination is a known issue (Stow et al., 2004; Gamon et al., 2013). The cloud detection algorithm developed by Gómez-Chova et al. (2008c) and implemented within

the CHRIS/PROBA Toolbox provides probability and cloud abundance for each pixel (instead of a binary mask) (Gómez-Chova et al., 2008c). It takes advantage of the number of spectral bands, the high spatial resolution, and the central wavelength positions of the bands to fully characterize spectral features within each image (cloud and non-cloud). The algorithm implements six steps: (1) *image preprocessing* – CHRIS images are first corrected for illumination effects caused by sun-target-sensor geometry and topography; (2) *feature extraction* – geophysical features are extracted to increase separability between clouds and ground cover; (3) *image clustering* – an unsupervised clustering is used to separate clouds from ground cover; (4) *cluster labelling* – resulting clusters are subsequently labeled into geophysical classes (i.e. the identification of cloud clusters); (5) *spectral unmixing* – is applied to the segmented image components to produce an abundance map of cloud content for all pixels. The algorithm processing parameters used in this study were as follows: number of clusters = 14; number of iterations = 30; the random seed was set to 31415; near-infrared (NIR) brightness and whiteness were selected; and the use of atmospheric water vapour features and atmospheric oxygen features were used. The clusters that corresponded to clouds were manually selected (typically only one class) by visual inspection, and finally the algorithm was set to process a probabilistic cloud mask. Probabilistic cloud masks were used for all atmospheric corrections.

Atmospheric correction: The images were atmospherically corrected per the method described by Guanter et al. (2008). The interface between atmospheric and geometric correction was not established in the CHRIS/PROBA Toolbox at the time of use (Version 5). Thus, the elevation and topographic effects calculated from a georeferenced digital elevation model were not considered in the CHRIS/PROBA atmospheric correction module (ACM) used in this study. The CHRIS/PROBA ACM is based around the MODerate resolution TRANsmittance (MODTRAN4)

atmospheric radiative transfer code (Berk et al., 2003; Guanter et al., 2008). MODTRAN4 is used for the generation of the look-up-table (LUT) that provides the atmospheric parameters used in the inversion of the CHRIS/PROBA top-of-atmosphere (TOA) radiance measurements for retrieval of surface reflectance values. MODTRAN4 was implemented into the CHRIS/PROBA ACM due to its recognized treatment of atmospheric scattering and absorption with respect to aerosols (i.e. aerosol optical thickness, AOT) and water vapour (i.e. columnar water vapour, CWV) (Guanter et al., 2008). The LUT used in the inversion depends on six free input parameters: VZA, SZA, RAA, surface elevation, AOT at 550 nm, and CWV. The atmospheric profile is defined by the mid-latitude summer atmosphere, the aerosol type is fixed to the continental model, and the ozone concentration is fixed to 7.08 g/m^2 . It should be noted that the atmosphere model used in the CHRIS/PROBA ACM could not be altered to a more preferred sub-Arctic summer profile (i.e. the software could not be edited). The CHRIS/PROBA ACM algorithm proceeds as follows. (1) *Spectral calibration*: The first step is the evaluation of instrument spectral calibration (i.e. spectral shifts due to sensor degradation, smile effect, etc.) and the subsequent removal of errors. The O_2 absorption feature centered at 760 nm is used as reference for the spectral calibration. (2) *Retrieval of AOT*: The total aerosol loading is parameterized by the AOT at 550 nm. AOT is calculated through the inversion of TOA radiance values to find the greatest contrast between green vegetation and bare soil pixels. Alternatively, the ACM allows the user to specify AOT values. As there were generally no nearby installations (e.g. airports) from which AOT values could be derived, an attempt was made to use Moderate Resolution Imaging Spectro-radiometer (MODIS) MOD04_L2 AOT values. However, poor surface reflectance results led to their rejection and default algorithm parameters were used instead. The default algorithm parameters allow for the retrieval AOT from the inversion of the LUT. (3) *Retrieval of CWV*: Columnar water vapour

retrieval makes use of the water vapour absorption centered at 940 nm (left wing/side) and the 860 to 890 nm region which is free from water vapor absorption. Although the CWV parameter is automatically calculated by the ACM, it is possible to enter a user specified measurement. Again, MODIS MOD05_L2 CWV values were tried but poor surface reflectance results led to their rejection and use of default values. (4) *Retrieval of surface reflectance*: The derivation of surface reflectance is performed during CWV retrieval, as the atmospheric parameters calculated for the inversion of the CWV for each pixel are also used to invert the MODTRAN4 LUT for surface reflectance. Each of the reflectance images were further refined for adjacency effects, which are caused by photons reflected by various targets within the image and scattered by the atmosphere into the sensor's instantaneous field of view. The final step in the atmospheric correction was the removal of systematic errors in surface reflectance, a step that is typically called recalibration or spectral polishing. During the atmospheric correction process, errors can arise due to problems with instrument gain coefficients and inaccurate radiative transfer simulations within the atmosphere. Because of a known error where negative surface reflectance values are commonly retrieved after the implementation of the CHRIS/PROBA ACM (e.g. Stagakis et al., 2010; Verrelst et al., 2008), band 1 (centred at 411 nm) was discarded from the analysis.

An attempt was made to implement a second atmospheric correction algorithm for comparison. The empirically based Quick Atmospheric Correction (QUAC) was applied to all CHRIS/PROBA imagery using ENVI version 5.3 (Bernstein et al., 2012). It is an empirical correction that determines atmospheric correction parameters directly from the observed pixel spectra within a scene without the use of any additional information related to the atmosphere (e.g. AOT or CWV) or sun-target-sensor geometry (Bernstein et al., 2012). Even if a sensor does not possess proper radiometric calibration settings (gains/offsets), or if the solar illumination intensity is unknown,

QUAC can still retrieve reasonably accurate reflectance spectra (within 10%) if the following conditions are met: (1) there are at least 10 diverse materials in a scene, and (2) there are sufficiently dark pixels in a scene to allow for a good estimation of the baseline spectrum (Bernstein et al., 2012). Processing spectroscopic images with QUAC is typically much faster compared to more complex radiative transfer codes/methods.

Geometric correction/orthorectification: All CHRIS/PROBA M1 multi-angle images were orthorectified using the rigorous Optical and Radar Satellite Math Model developed by Toutin (Toutin et al., 1992; Toutin, 2004; Poli and Toutin, 2012). It is based on the collinearity condition where a ground point, its position in the optical plane and its position on the image plane should be collinear; using multiple points as reference, a transformation between the image space and ground space can be generated (PCI Geomatics, 2014). An in-depth description of the Toutin model is provided elsewhere (Toutin, 2004). The Toutin model describes the physical approximation of the viewing geometry and distortions generated during the image formation and considers such parameters as: (1) satellite position, velocity, and orientation; (2) sensor orientation, integration time, and field of view; (3) the earth geoid, ellipsoid, and relief; and (4) the cartographic projection (PCI Geomatics, 2014). The Toutin model is quick to implement as few ground control points (GCPs) are generally needed for accurate orthorectification in flat terrain (PCI Geomatics, 2014); however, mountainous areas can require additional GCPs. An example of the CHRIS/PROBA parameters implemented into the model are as follows (parameters were changed for each image given the specific image view geometry and platform position): (1) across track angle: 0° , (2) along track angle: 0° ; (3) instantaneous field of view: 0.0000597 rad; (4) altitude: 586000 m; (5) period: 96.97 minutes; (6) actual eccentricity: 0.0082774; (7) actual inclination 97.84° ; (8) ellipsoid: WGS 84. Each of the image and sensor parameters needed to run the model

was obtained from the image metadata. A high-resolution TanDEM-X digital elevation model (DEM) was used for the orthorectification process (provided by the German Aerospace Centre). TanDEM-X DEM has an approximate spatial resolution of ~12 m (0.4 arcsecond at the equator) with an absolute horizontal accuracy of <10 m, an absolute vertical accuracy of <10 m, and a relative vertical accuracy of ~2-4 m. GCPs were selected using visual analysis of pan-sharpened Landsat 8 imagery.

The results of the orthorectification, shown in Table 38, demonstrate that, as expected, nadir imagery was the most accurately rectified with an average x,y positional error of approximately ~13.05 m. The most extreme VZAs produced the greatest degree of positional error; for example -55° had a mean positional error of 21.62 m. The sites with the least overall accuracy occurred in mountainous terrain. For example, Banks Island, considered relatively flat, produced a mean positional error of 10.58 m, whereas the Richardson Mountains (2013 and (2014) images produced positional accuracies of 22.46 m and 21.44 m, respectively. Despite these variations, all orthorectified images had sub-pixel accuracy (<34 m).

Table 38 Average x,y positional error for CHRIS/PROBA ortho-rectified images. All measurements are in meters.

<i>View Zenith Angle</i>	<i>Herschel Island (2011)</i>	<i>Banks Island (2012)</i>	<i>Richardson Mountains (2013)</i>	<i>Richardson Mountains (2014)</i>	<i>Average RMSE</i>
0°	10.29	9.77	17.48	14.65	13.05
+36°	23.00	18.81	11.31	19.19	18.08
-36°	7.85	5.28	25.94	25.01	16.02
+55°	22.97	5.62	25.10	21.99	18.92
-55°	14.22	13.42	32.47	26.38	21.62
<i>Average RMSE</i>	15.67	10.58	22.46	21.44	17.54

Finally, spectra from the ortho-rectified CHRIS/PROBA ACM and QUAC surface reflectance products were extracted at each field plot and compared to the ground-level spectral measurements

to determine the spectral fidelity and accuracy of the space borne measurements. Correlation tests between CHRIS/PROBA ACM and QUAC surface reflectance products and field spectroscopy were performed using cross-correlation analysis and RMSE (Equation 22) (Sykioti et al., 2011).

7.2.5. Parametric regression (based on vegetation indices): SR and ROSAVI

Vegetation indices (VIs) were computed from the multi-angle CHRIS/PROBA M1 surface reflectance products and compared, based on their linear relationship, to the field-based biochemical and biophysical measurements (i.e. LCC, PAI_e, and CCC_e). Each observation angle was processed as an individual set of reflectance measurements and each of the following analyses was applied separately for the different VZAs. The VI analysis was categorized into two approaches: (1) analysis of a multi-band VI based on a common spectral formulation, the simple ratio (SR; Equation 21) (Birth & McVey, 1968), and (2) analysis of a predefined narrowband VI, the revised optimized soil adjusted vegetation index (ROSAVI; Table 24) (Wu et al., 2008). The selection of these VIs was based on a previously conducted field spectroscopy analysis (Chapter 5), where a comprehensive list of VIs found in the remote sensing literature were investigated for their overall robustness for predicting LCC, PAI_e, and CCC_e across a latitudinal gradient and across angular reflectance measurements. Although VI analyses have been completed in the Arctic (e.g. Buchhorn et al., 2013; Bratsch et al., 2016; Liu et al., 2017), there has not been a comprehensive assessment of narrowband VIs for predicting and retrieving vegetation biochemical and biophysical variables from a space-borne multi-angle imaging spectrometer.

As in the field scale analysis of Chapter 5, in this study all possible two band SR combinations were computed. For ROSAVI, as in Chapter 5, since it is defined using reflectance values of bands 705 nm and 750 nm, the 703 nm and 748 nm wavelengths of the CHRIS/PROBA were used. Selection of the optimal bands within the multi-band VI (i.e. SR) was conducted by calculating

the weighted mean centre of the spectral space using the r^2 as the weighting. For the two VIs, detailed analysis of r^2 and predictive performance (RMSE) across all these data configurations is presented in the Results. The Normalized RMSE or NRMSE (RMSE/range of measured data) (Darvishzadeh et al., 2008a) was used to compare the overall model predictions for the individual and combined variables (i.e. LCC, PAI_e, CCC_e) at the various VZAs for the selected VIs. An NRMSE of 0.10 (10%) is commonly regarded as an accuracy threshold in an operational context (Drusch et al., 2012); however, all NRMSE values were considered.

7.2.6. Non-parametric regression: Gaussian Processes Regression (GPR)

The GPR Band Analysis Tool (GPR-BAT) algorithm, as previously described in Chapters 2 and 5, was implemented to analyze the CHRIS/PROBA surface reflectance datasets described above. The spectral data were processed systematically to assess: (1) the overall performance of the GPR algorithm, measured in terms of r^2 and RMSE, for predicting LCC, PAI_e, and CCC_e at the various VZAs and field sites, and (2) the optimal wavelength regions for the field variables in question (LCC, PAI_e, and CCC_e) across the various VZAs and field site. The GPR-BAT algorithm was programmed to remove one band at a time. The NRMSE was later computed to compare the overall GPR model predictions for the individual and combined variables (i.e. LCC, PAI_e, CCC_e) at the various VZAs. Finally, all modelled prediction results (SR, ROSAVI, and GPR) were ultimately compared using the NRMSE to assess overall model accuracy.

As in the empirical field-scale study (Chapter 5), validation of the regression models (i.e. SR, ROSAVI, GPR) was based upon a 10-fold ($k=10$) cross-validation procedure and was implemented in the ARTMO (Automated Radiative Transfer Models Operator) software package (Verrelst et al., 2012c; Rivera et al., 2014a,b). All empirical model evaluation metrics (r^2 , RMSE, NRMSE)

correspond to the k -fold cross-validation procedure and are thus denoted as such (e.g. r^2_{cv} , $RMSE_{cv}$, $NRMSE_{cv}$).

7.2.7. Physically based radiative transfer modelling: PROSAIL and LMA inversion

The PROSAIL modelling and LMA inversion process as described in Chapters 2 and 6 was implemented using the same procedure given in the Chapter 6 field-scale study. The initial starting input parameters and parameter ranges for the inversions were implemented using two approaches: (a) use of the mean values and original full range for each of the measured field variables found across all sites, and for unknown parameters, based on accepted values found in the literature as discussed in Chapter 6 (Table 33); (b) use of the mean values and constrained ranges (i.e. within one standard deviation) of the inverted PROSAIL parameters that were found in the field scale analysis of Chapter 6 (Table 36: Column “Mean Modelled Values (ASD)” and “Standard deviation (ASD)”). The measured parameter ranges (e.g. chlorophyll) used in the constrained inversion were based upon the originally measured parameter space. The inverted PROSAIL top-of-canopy (TOC) spectral reflectance and leaf and canopy parameters were compared to measured field variables (spectra, LCC, PAI_e , and CCC_e) using the coefficient of determination (r^2) and the RMSE. Finally, the overall physical modelling results were compared to the empirical modelling results using the NRMSE. All physical model evaluation metrics (r^2 , RMSE, NRMSE) were not evaluated using the k -fold cross-validation procedure.

7.3. Results

The results of the CHRIS/PROBA preprocessing and modelling are presented in the following order: (1) comparison of satellite derived surface reflectance and ground measured reflectance, (2) narrowband parametric regression using SR and ROSAVI, (3) non-parametric regression using GPR, and (4) LMA inversion of PROSAIL.

7.3.1. Comparison of satellite derived surface reflectance and ground measured reflectance

A comparison of the CHRIS-derived surface reflectance products showed that the ACM radiative transfer based corrections produced nominally better results than the QUAC empirically based corrections when compared to ASD reference ground spectra (Figure 69). The CHRIS/PROBA ACM produced overall mean RMSE values of 0.033 (min=0.01, max=0.06), whereas the QUAC correction produced an overall mean RMSE of 0.034 (min=0.01, max=0.07) – a nominal difference. An examination of both corrections (Figure 69) reveals that the QUAC algorithm is surprisingly robust for an algorithm that does not use parameterization; however, it tended to perform worse than ACM in the near-infrared regions at all sites except Richardson Mountains 2014, where the opposite occurred. The discrepancies between the CHRIS/PROBA surface reflectance products and the ground based spectral measurements are likely due to several factors: (1) an inconsistency between field work and image acquisition dates and times; (2) the ground-based spectral measurements taken at slightly different VZAs and during times with slightly different SZAs; (3) the reflectance products derived from the CHRIS/PROBA acquisitions are the product of the atmospheric RTM assumptions; and (4) reflectance products derived from the CHRIS/PROBA sensor are from a much larger and thus different physical surface (i.e. this may provide a better representation of TOC reflectance). All attempts were made to conduct fieldwork during planned acquisition times. It is also possible that the estimated metadata values produced erroneous results with the CHRIS/PROBA ACM LUT inversions. Given the above, and the marginally better ACM results, it was decided to use the CHRIS/PROBA ACM reflectance products in the empirical and physically based vegetation modelling.

Figure 69 Comparisons of CHRIS/PROBA ACM, and QUAC atmospheric correction spectra to ground-based multi-angle ASD spectra. All Herschel Island ground spectra were acquired at nadir, so off-nadir ground spectra are not shown for that site.

The assessment of field-based reflectance spectra can be found in Chapter 5. Given that other studies have characterized Arctic tundra reflectance based on the stratification of ground moisture, potential of hydrogen (pH), and plant community composition (Buchhorn et al., 2013; Bratsch et al., 2016; Liu et al, 2017), the focus here was on describing the generalized reflectance anisotropy based on the overall mean reflectance values measured across each field site and VZA as measured from the satellite platform irrespective of ground condition, as was completed for the field-based spectral measurements. The following sections provide brief descriptions CHRIS/PROBA reflectance signatures and the assessed coefficient of variation as related to: (1) the visible wavelength region (VIS, 442-691 nm), (2) the red-edge (RE, ~691-755 nm), and (3) the near-infrared (NIR, 722-997 nm). Figure 70 shows a comparison of the multi-angle CHRIS/PROBA M1 ACM products that were used for the study. Figure 71 shows the coefficient of variation for each of the multi-angle CHRIS/PROBA M1 ACM TOC reflectance products.

Figure 70 Comparison of multi-angle CHRIS/PROBA ACM modelled TOC reflectance for all four field sites.

Figure 71 Comparison of the coefficient of variation for the multi-angle CHRIS/PROBA ACM modelled TOC reflectance products for all field sites.

In the VIS wavelength region, all sites showed an overall increasing trend in reflectance values progressing from 442 nm to 691 nm with damped chlorophyll absorption in the red wavelengths (~670 to 680 nm), like those reported in the field-based study (Chapter 5) and in comparable Arctic field-based spectroscopy studies (Buchhorn et al., 2013; Bratsch et al., 2016; Liu et al, 2017). Similarities between the field and remote sensing spectra included: (a) a gradual increase in VIS reflectance for the high Arctic (e.g. Banks Island), where significant amounts of dry bare soil and senescent vegetation occur; (b) increased absorption in the pigment (chlorophyll) absorption regions at lower latitudes, where smaller gap fractions and greater quantities of chlorophyll/leaves occur. Multi-angle VIS reflectance showed a standard response across all sites: backscatter reflectance (e.g. -55° and -36°) was generally greater at all wavelengths than at nadir (0°) and in the forward direction ($+55^{\circ}$ and $+36^{\circ}$). On the other hand, forward scatter showed an atypical response at several of the sites as compared to the ground based multi-angle reflectance measurements. For example, Herschel Island forward scatter reflectance values were similar but slightly less than nadir values when it was expected that they would be larger than nadir values.

This was not surprising since the RAA values of $+55^\circ$ and $+36^\circ$ were almost identical to the nadir RAA value (121.3° , 128.4° , 128.6° , respectively), and furthermore, the nadir VZA was $+15.12^\circ$. This atypical response was also recorded at the Banks Island site, however, the nadir RAA value (50.0°) was in the backscatter angular trajectory (i.e. $< 60^\circ$), so this may explain the elevated values. Lower forward scatter values were also observed for $+36^\circ$ at the Richardson Mountains (2013) site; nadir measurements at this site had a RAA of greater than 60° (97.84°) and a VZA greater closer to the forward scatter measurements ($+21^\circ$). It is possible that reflectance values are erroneous since metadata values were estimated in some instances, thus potentially contributing to inversion errors of the MODTRAN4 LUT.

The coefficient of variation of reflectance values showed a similar response to the field-scale spectra across all sites. Generally, reflectance values at lower wavelengths (e.g. ~ 442 nm to ~ 530 nm) showed the highest degree of variability, with a pronounced dip in variability at ~ 551 nm (i.e. peak green reflectance), and a subsequent increase in variability at ~ 680 nm (i.e. pigment absorption) at all VZAs. Explanations for the observed variability have been provided in Chapter 5, and relate to such factors as: (1) differing acquisition times and angles, (2) sampling gradients, (3) leaf and canopy chemical and structural differences (as they relate to latitude, seasonality, weather, and phenology), and (4) sensor noise. Finally, like the field-scale analysis, variability in relation to VZA showed no clear tendency (i.e. forward and backscatter were both variable across the field sites at all VIS regions). The variability observed in the Richardson Mountains 2014 as compared to the previous field season may be due to the seasonal weather patterns (i.e. plant phenology or soil/sphagnum/understory moisture) or to the time of year sampling was conducted (i.e. plant phenology/senescence).

The results for the RE wavelength region are like those reported at the ground level (Chapter 5). The RE had the greatest slope at lower latitudes in regions with greater overall quantities of canopy chlorophyll content and green leaf matter per unit area (i.e. CCC_e), thus providing a greater difference between red absorption and NIR reflectance as compared to more northerly sites. The shallowest RE slope was observed in the most northern site (Banks Island). RE backscatter reflectance (-55° and -36°) was greater than at nadir and in the forward direction. An exception occurred at two sites: (1) the Herschel Island site, where, as previously stated, nadir reflectance values were greater than both forward scatter values; and (2) the Richardson Mountains site, where nadir reflectance was greater than the $+36^{\circ}$ VZA but not greater than for the $+55^{\circ}$ VZA. Another interesting result was that $+55^{\circ}$ VZA reflectance values for the Richardson Mountains (2014) were almost identical to those for -55° VZA. The coefficient of variation of reflectance values showed a similar response to the field-scale spectra across all sites and did not show any clear tendency when examined with respect to VZA. Reasons for the low degree of variability observed in the RE region maybe due to leaf/plant structure that persists after initial development as was previously discussed in Chapter 5.

In the NIR wavelength regions, all vegetation plots showed overall low nadir reflectance (<0.5), with the lowest overall reflectance values occurring in the most northern location (Banks Island). Similar low nadir reflectance was reported at the field-scale (Chapter 5) and has been reported in similar studies within the Arctic e.g. (<0.4) (Bratsch et al., 2016; Buchhorn et al., 2013; Davidson et al., 2016; Ulrich et al., 2009; Liu et al., 2017). Like the field-based spectra, the surface reflectance values from the CHRIS/PROBA sensor did not produce the typical green vegetation NIR reflectance plateau (e.g. Bratsch et al., 2016; Buchhorn et al., 2013; Davidson et al., 2016; Ulrich et al., 2009; Liu et al., 2017) and may be attributed to low vegetation height/structure and

low green leaf area. NIR reflectance values at nadir (0°) were among the lowest for all sites, and as was anticipated, backscatter measurements (e.g. -55° and -36°) produced the greatest reflectance. NIR results that were atypical occurred in the following situations: (1) Herschel Island forward scatter NIR values ($+55^\circ$ and $+36^\circ$) were less than nadir values, (2) Richardson Mountains (2013) $+36^\circ$ NIR values were less than nadir values, and (3) Richardson Mountain (2014) $+55^\circ$ NIR values were nearly identical to -55° NIR values even though RAA values were 111.8° and 33.49° respectively.

Coefficient of variation values for all sites indicate that the lowest and most stable reflectance variability exists in this spectral region for all field sites and may be an overall indication of leaf and canopy structure, as observed in the ground spectra. The observed differences in NIR variability for the Richardson Mountains between seasons (2013 and 2014) may be due to the reasons provided for the lower wavelength spectral regions (i.e. phenology and weather). No obvious trends for the coefficient of variation is observable when examined in the context of VZA; however, -55° reflectance values were among the highest for three of the four sites.

7.3.2. Parametric regression: SR and ROSAVI

The results of the cross-validated VI based parametric regression analyses are presented in Table 39. Cross-validated correlation coefficient (r^2_{cv}) values are presented using a red/white/blue colour ramp to highlight poor (blue, $r^2_{cv}=0$) to median (white, $r^2_{cv}=0.5$) to optimal results (red, $r^2_{cv}=1$) and are presented with associated error metrics ($RMSE_{cv}$). Overall, it was shown that the multi-band SR VI (mean $r^2_{cv}=0.53$) outperformed the predefined narrowband ROSAVI (mean $r^2_{cv}=0.48$) across all field sites, VZAs, and vegetation variables. The Richardson Mountains 2014 -55° VZA was removed from the empirical cross-validation analysis to due to the lack of field plots within the image ($n=11$).

Table 39 Parametric linear regression modelling results for SR and ROSAVI retrievals using the CHRIS/PROBA ACM surface reflectance data. Plotted relationships are bolded and marked with an asterisk.

Colour Scale (r^2_{cv})			CHRIS/PROBA M1: Multi-Band				Predefined Narrowband	
0 1			Simple Ratio (SR)		SR – Best bands		ROSAVI	
Location	VZA	Variable	r^2_{cv}	RMSE _{cv}	B1 (nm)	B2 (nm)	r^2_{cv}	RMSE _{cv}
Herschel Island (2011)	0°	LCC	0.42	3.93	581	572	0.35	4.29
		PAI _e	0.52	0.19	742	735	0.43	0.21
		CCC _e	0.57	0.07	955	833	0.46	0.08
	-36°	LCC	0.38	3.49	510	530	0.33	4.20
		PAI _e	0.36	0.21	490	500	0.34	0.23
		CCC _e	0.45	0.08	955	859	0.39	0.09
	-55°	LCC	0.29	4.02	581	572	0.20	4.92
		PAI _e	0.39	0.22	530	520	0.22	0.26
		CCC _e	0.46	0.08	530	510	0.29	0.10
	+36°	LCC*	0.47	3.87	471	461	0.38	4.18
		PAI _e	0.40	0.19	530	551	0.40	0.21
		CCC _e	0.52	0.07	530	551	0.45	0.08
	+55°	LCC	0.37	3.98	530	540	0.16	4.81
		PAI _e	0.38	0.23	500	481	0.29	0.26
		CCC _e	0.35	0.09	530	551	0.38	0.10
Banks Island (2012)	0°	LCC	0.74	5.18	481	915	0.70	6.37
		PAI _e *	0.87	0.10	703	530	0.83	0.11
		CCC _e	0.85	0.04	490	551	0.79	0.05
	-36°	LCC	0.58	5.96	442	915	0.57	7.12
		PAI _e	0.75	0.12	510	581	0.71	0.13
		CCC _e	0.73	0.05	530	540	0.65	0.06
	-55°	LCC	0.62	7.03	442	925	0.61	8.26
		PAI _e	0.70	0.14	762	755	0.67	0.16
		CCC _e	0.57	0.06	762	755	0.55	0.07
	+36°	LCC	0.60	6.78	530	709	0.51	7.22
		PAI _e	0.80	0.12	703	471	0.71	0.13
		CCC _e	0.76	0.05	716	471	0.68	0.06
	+55°	LCC	0.76	6.28	442	691	0.66	7.97
		PAI _e	0.84	0.10	520	581	0.76	0.14
		CCC _e	0.82	0.04	520	581	0.72	0.06
Richardson Mountains (2013)	0°	LCC	0.34	4.27	777	785	0.37	5.30
		PAI _e	0.70	0.12	748	716	0.65	0.16
		CCC _e	0.52	0.07	581	561	0.57	0.09
	-36°	LCC	0.12	4.32	965	886	0.40	6.13
		PAI _e	0.51	0.14	997	672	0.26	0.15
		CCC _e	0.28	0.07	895	965	0.27	0.08
	-55°	LCC	0.27	4.46	877	965	0.33	5.43
		PAI _e	0.55	0.13	716	691	0.69	0.13
		CCC _e	0.48	0.06	965	859	0.37	0.08
	+36°	LCC	0.50	4.37	905	976	0.25	5.06
		PAI _e	0.68	0.14	716	709	0.59	0.15
		CCC _e *	0.51	0.07	915	976	0.50	0.08
	+55°	LCC	0.34	4.36	940	800	0.27	5.39
		PAI _e	0.65	0.11	561	572	0.64	0.13
		CCC _e	0.27	0.07	561	551	0.32	0.08
Richardson Mountains	0°	LCC	0.36	2.15	800	833	0.46	2.14
		PAI _e	0.43	0.31	631	686	0.44	0.41

(2014)		<i>CCC_e</i>	0.39	0.14	631	686	0.44	0.17
	-36°	<i>LCC</i>	0.50	2.06	572	540	0.54	2.11
		<i>PAI_e</i>	0.69	0.28	762	785	0.28	0.44
		<i>CCC_e</i>	0.66	0.13	762	777	0.29	0.18
	+36°	<i>LCC</i>	0.46	2.12	850	785	0.54	2.10
		<i>PAI_e</i>	0.41	0.30	895	868	0.38	0.40
		<i>CCC_e</i>	0.40	0.13	895	868	0.39	0.17
	+55°	<i>LCC</i>	0.50	1.63	850	833	0.45	3.26
		<i>PAI_e</i>	0.55	0.33	955	859	0.84	0.39
		<i>CCC_e</i>	0.82	0.13	500	590	0.70	0.17
	<i>All sites</i>	<i>Overall</i>	0.53	-	664	683	0.48	-
	<i>All</i>	<i>LCC</i>	0.45	4.22	620	754	0.43	5.07
	<i>All</i>	<i>PAI_e</i>	0.59	0.18	686	644	0.53	0.22
	<i>All</i>	<i>CCC_e</i>	0.55	0.08	676	666	0.48	0.10
	0°	<i>LCC</i>	0.47	3.88	619	798	0.47	4.53
	-36°	<i>LCC</i>	0.40	3.96	539	702	0.46	4.89
	-55°	<i>LCC</i>	0.39	5.17	576	847	0.38	6.20
	+36°	<i>LCC</i>	0.51	4.29	681	735	0.42	4.64
	+55°	<i>LCC</i>	0.49	4.06	648	717	0.39	5.36
	0°	<i>PAI_e</i>	0.63	0.18	711	651	0.59	0.22
	-36°	<i>PAI_e</i>	0.58	0.19	690	649	0.40	0.24
	-55°	<i>PAI_e</i>	0.55	0.16	691	678	0.53	0.18
	+36°	<i>PAI_e</i>	0.57	0.19	711	627	0.52	0.22
	+55°	<i>PAI_e</i>	0.61	0.19	627	626	0.63	0.23
	0°	<i>CCC_e</i>	0.58	0.08	648	645	0.57	0.10
	-36°	<i>CCC_e</i>	0.53	0.08	741	738	0.40	0.10
	-55°	<i>CCC_e</i>	0.50	0.07	756	713	0.40	0.08
	+36°	<i>CCC_e</i>	0.55	0.08	751	680	0.51	0.10
	+55°	<i>CCC_e</i>	0.57	0.08	519	576	0.53	0.10
	0°	<i>All</i>	0.56	-	664	689	0.54	-
	-36°	<i>All</i>	0.50	-	668	694	0.42	-
	-55°	<i>All</i>	0.48	-	682	736	0.44	-
	+36°	<i>All</i>	0.54	-	715	678	0.48	-
	+55°	<i>All</i>	0.55	-	596	636	0.52	-

Visualization of the results based on vegetation variable, VZA, and geographic location can be seen in Figure 72. SR produced overall higher mean r^2_{cv} values for *PAI_e* ($r^2_{cv}=0.59$, $RMSE_{cv}=0.18$) than for *LCC* ($r^2_{cv}=0.45$, $RMSE_{cv}=4.22$) or *CCC_e* ($r^2_{cv}=0.55$, $RMSE_{cv}=0.08$), and equally so for the ROSAVI analyses (*LCC*, $r^2_{cv}=0.43$, $RMSE_{cv}=5.07$; *PAI_e*, $r^2_{cv}=0.53$, $RMSE_{cv}=0.22$; *CCC_e*, $r^2_{cv}=0.48$, $RMSE_{cv}=0.10$). These results match those of the field-scale analysis (Chapter 5), where the highest r^2_{cv} values were achieved for *PAI_e* followed by *CCC_e* and then *LCC*. Possible reasons for this were discussed in Chapter 5 and include the detectability of plant greenness/structure as compared to pigment quantities occurring at finer spatial scales. The synthetic variable, *CCC_e*,

achieved better results than LCC at all sites for both SR and ROSAVI ($CCC_e r^2_{cv}=0.48$ vs. LCC $r^2_{cv}=0.43$). Better results for PAI_e (or LAI) and CCC_e as compared to LCC have been reported in similar studies (e.g. Darvishzadeh et al., 2008a). The VZA that produced the best mean results for all three vegetation variables was 0° (SR $r^2_{cv}=0.56$ and ROSAVI $r^2_{cv}=0.54$), while the $+55^\circ$ VZA produced the second-best results (SR $r^2_{cv}=0.54$ and ROSAVI $r^2_{cv}=0.52$). This result contrasts that of the field-scale analysis, where the best overall results were achieved at -55° . The variability of the predicted vegetation variables in relation to VZA can be seen in Figure 72 (top right).

When VI results were stratified per geographic locations, similar regionally based results are reported here as for the field scale analyses. As in the field scale analyses, Banks Island (2012) produced the best overall predictions for all vegetation (Figure 72, bottom left). The r^2_{cv} values between the measured and predicted variables for Banks Island were high for all vegetation variables (e.g. 0° VZA: LCC, $r^2_{cv}=0.74$, $RMSE_{cv}=5.81$; PAI_e , $r^2_{cv}=0.87$, $RMSE_{cv}=0.10$; CCC_e , $r^2_{cv}=0.85$, $RMSE_{cv}=0.04$). All other field sites produced poorer predictive relationships between the cross-validated VIs and LCC, PAI_e , and CCC_e . Possible reasons for this were discussed in Chapter 5 and include the large spatial variation observed for LCC, PAI_e , and CCC_e values on Banks Island.

Figure 72 Boxplot comparison of SR and ROSAVI cross-validated r^2_{cv} for locations, look angles, vegetation variables, and vegetation variable/angles. Boxplots show the interquartile range with factor of 1.5; outliers are displayed with a +.

The multi-band SR VI produced a wide range of optimal spectral bands for the various datasets (Table 39). As in the field scale analysis, the globally-optimal bands were calculated using a weighted-mean, calculated using the associated r^2_{cv} values as the weighting. Optimal weighted mean band selections for LCC at all VZAs and field sites were clustered around the VIS pigment absorption regions for chlorophyll ($BI = \sim 539$ to 681 nm) and within the RE and NIR regions

typical of healthy vegetation ($B2 = \sim 717$ to 847 nm). Optimal weighted bands for PAI_e were more overlapping with $B2$ centred more in the visible than the RE ($B1 = 627-711$ nm; $B2 = 626-678$ nm). Optimal bands for CCC_e were broader than for both LCC and PAI_e , with $B1$ extending from the blue-green to near the top of the RE, and $B2$ from the green to RE ($B1 = 519-756$ nm; $B2 = 576-738$ nm). Band selections for LCC, PAI_e , and CCC_e match very closely to those bands reported at the field scale, and other studies that have measured similar green-based vegetation variables, such as percent green vegetation cover ($\sim 680-872$ nm) (Liu et al., 2017) and biomass ($\sim 680-872$ nm) (Buchhorn et al., 2013).

To provide a better visualization of optimal band selections within their associated spectral space, two-band selections were graphed with their accompanying r^2_{cv} value (Figure 73). Surface-map visualizations allow for a qualitative interpretation of spectral space and an assessment of the optimal regions that are of greater importance to the variable in question (as shown in Chapter 5). These maps are not plotted using the weighted mean of the spectral space, but highlight the same spectrally important regions. In Figure 73, all variables demonstrated a high degree of spectral variability with respect to VZA; however, several patterns are evident as optimal spectral regions are generally quite distinct from other regions in this Figure. When examining the overall combined variables, it is evident that optimal band selection regions shift with VZA. For LCC, there appears to be distinct spectral regions that produce above average results for all VZAs that are centred within $B1 \sim 442-551$ nm and $B2 \sim 700-950$ nm, a result that is similar to the field-based result (Chapter 5). PAI_e and CCC_e , in contrast, appear to have very defined small optimal spectral areas that vary with VZA, except at -36° where there appears to be a larger optimal spectral region.

Figure 73 All 2-band optimal variable selections for the SR VI (x and y axes) and their associated r^2_{cv} values (z-axis) for each of the view angles (at plot scale, not weighted). One or more distinct optimal spectral regions for each field variable and VZA are evident in each graph.

Figure 74 Weighted band selections for each vegetation variable and view zenith angle for SR VI. Optimal bands selected in the SR optimization show that wavelength selections generally show no distinct patterns from backscatter to forward scatter.

When optimal SR bands are plotted with respect to VZA, a very weak trend emerges that is contrary to that reported at the field-scale in Chapter 5 (Figure 74). The SR CHRIS/PROBA band selections decrease in wavelength as VZA progresses from backscatter to forward scatter, with the exception being Band 1 predictors for LCC. However, the amount of variability observed in the band selections may also be the result of chance (natural variability) or noise/error encountered in

the measured reflectance signals, as was discussed in Chapter 5. The difference between the field scale and the remote sensing scale may be due to two factors: (1) the field scale analysis is not capturing reflectance as it appears at the satellite scale (i.e. the surface may behave differently from the remote sensing scale), and (2) the field scale reflectance measurements were integrated over several hours of sun positions and conditions, whereas the sun position of the remote sensing acquisition remains stationary.

Scatter plots showing some of the optimal measured vs. modelled relationships for select field sites (LCC, Herschel Island +36°; PAI_e, Banks Island 0°; CCC_e, Richardson Mountains 2013 +36°) are displayed in Figure 75. Calibration equations established in the SR and ROSAVI regression analyses were subsequently used to map LCC, PAI_e, and CCC_e with various CHRIS/PROBA images (Figure 76). Mapped variables also demonstrate that the predefined narrowband ROSAVI tended to have higher variance in predicted values of each variable as well as a larger positive bias (intercept of regression equation) as compared to the SR.

Figure 75 Scatterplots showing SR and ROSAVI measured vs. predicted relationships for example field sites and VZAs.

Figure 76 SR and ROSAVI predictive maps for various field sites: Herschel Island 2011 (top), Banks Island 2012 (middle), and Richardson Mountains 2013 (bottom). Wavelengths used for each retrieval match the regressions in Figure 74 and represent optimal spectral regions.

7.3.3. Non-parametric regression: Gaussian Processes Regression (GPR)

The results of the GPR analyses are presented in Table 40. Cross-validated correlation coefficient (r^2_{cv}) values are presented using a red/white/blue colour ramp to highlight poor (blue, $r^2_{cv}=0$) to median (white, $r^2_{cv}=0.5$) to optimal results (red, $r^2_{cv}=1$) and are presented with associated error metrics ($RMSE_{cv}$). Overall, results showed that GPR produced the highest correlation based results for each of the vegetation variables regardless of VZA and geographic location (mean $r^2_{cv}=0.59$). The best single variable (i.e. the last remaining predictor band) produced a mean $r^2_{cv}=0.44$ over the three vegetation variables, irrespective of VZA and geographic location.

Table 40 GPR-BAT results for CHRIS/PROBA ACM dataset for the best overall selected model and single best band model. Overall band selection results are shown for the best bands (highest predictive power) and highest ranked bands (most common band selected across all GPR models) from GPR-BAT analysis. Plotted relationships are bolded and marked with an asterisk.

Colour Scale (r^2_{cv})			CHRIS/PROBA M1					
0 1			Plot: Best Model		Plot: Best Band		Best Band	Overall Rank
Location	VZA	Variable	r^2_{cv}	$RMSE_{cv}$	r^2_{cv}	$RMSE_{cv}$	Wavelength (nm)	Wavelength (nm)
Herschel Island (2011)	0°	LCC	0.3	4.56	0.3	4.87	452	442
		PAI _e	0.39	0.22	0.29	0.25	742	742
		CCC _e	0.48	0.08	0.48	0.10	742	656
	-36°	LCC*	0.58	3.70	0.35	4.35	510	661
		PAI _e	0.58	0.19	0.45	0.27	755	556
		CCC _e	0.5	0.08	0.49	0.11	770	551
	-55°	LCC	0.53	4.36	0.53	4.36	735	722
		PAI _e	0.66	0.21	0.42	0.27	997	520
		CCC _e	0.66	0.07	0.39	0.11	471	515
	+36°	LCC	0.39	4.54	0.27	4.66	442	540
		PAI _e	0.37	0.21	0.36	0.22	742	709
		CCC _e	0.41	0.09	0.23	0.10	672	561
	+55°	LCC	0.35	4.89	0.13	5.08	461	471
		PAI _e	0.63	0.24	0.27	0.26	716	653
		CCC _e	0.6	0.10	0.17	0.12	551	676
Banks Island (2012)	0°	LCC	0.62	7.00	0.53	7.01	561	770
		PAI _e	0.84	0.11	0.81	0.13	461	728
		CCC _e	0.71	0.06	0.71	0.06	471	748
	-36°	LCC	0.63	5.37	0.48	7.70	520	490
		PAI _e	0.76	0.12	0.64	0.15	915	716
		CCC _e	0.69	0.06	0.64	0.06	915	703
	-55°	LCC	0.72	5.43	0.72	5.43	997	722
		PAI _e	0.62	0.16	0.59	0.17	510	965
		CCC _e	0.45	0.08	0.45	0.08	500	976
	+36°	LCC	0.53	8.88	0.14	11.05	561	603
		PAI _e	0.65	0.17	0.53	0.18	461	905
		CCC _e	0.6	0.07	0.51	0.07	442	755
	+55°	LCC	0.68	7.08	0.68	7.08	452	716
		PAI _e *	0.86	0.12	0.85	0.13	442	447
		CCC _e	0.83	0.05	0.83	0.05	442	722
Richardson Mountains (2013)	0°	LCC	0.52	5.06	0.31	5.16	672	616
		PAI _e	0.61	0.18	0.49	0.20	442	481
		CCC _e	0.6	0.10	0.23	0.11	691	481
	-36°	LCC	0.35	5.76	0.27	5.80	680	651
		PAI _e	0.52	0.20	0.3	0.22	672	561
		CCC _e	0.42	0.10	0.37	0.11	641	447
	-55°	LCC	0.58	4.98	0.42	5.77	672	486
		PAI _e	0.53	0.19	0.41	0.21	748	652
		CCC _e	0.62	0.09	0.48	0.11	481	490
	+36°	LCC	0.52	5.00	0.52	5.02	672	500
		PAI _e	0.61	0.18	0.51	0.20	442	461
		CCC _e	0.4	0.10	0.25	0.11	442	500
	+55°	LCC	0.74	5.53	0.25	5.53	735	540
		PAI _e	0.37	0.19	0.31	0.19	661	603
		CCC _e	0.57	0.10	0.39	0.10	672	686

<i>Richardson Mountains (2014)</i>	0°	<i>LCC</i>	0.71	2.30	0.19	2.30	686	706
		<i>PAI_e</i>	0.64	0.28	0.32	0.37	722	703
		<i>CCC_e*</i>	0.61	0.11	0.39	0.14	716	703
	-36°	<i>LCC</i>	0.54	1.92	0.21	2.57	716	471
		<i>PAI_e</i>	0.68	0.36	0.52	0.40	703	540
		<i>CCC_e</i>	0.62	0.16	0.3	0.20	703	481
	$+36^\circ$	<i>LCC</i>	0.71	2.23	0.09	2.30	748	686
		<i>PAI_e</i>	0.59	0.28	0.46	0.30	530	486
		<i>CCC_e</i>	0.59	0.12	0.48	0.13	530	684
	$+55^\circ$	<i>LCC</i>	0.8	2.24	0.64	2.64	510	641
		<i>PAI_e</i>	0.86	0.34	0.83	0.36	471	442
		<i>CCC_e</i>	0.77	0.14	0.76	0.14	965	680
<i>All sites</i>	<i>Overall</i>		0.59	-	0.44	-	628	623
	<i>All</i>	<i>LCC</i>	0.57	4.78	0.37	5.19	633	614
	<i>All</i>	<i>PAI_e</i>	0.62	0.21	0.49	0.24	627	618
	<i>All</i>	<i>CCC_e</i>	0.59	0.09	0.45	0.11	625	638
	0°	<i>LCC</i>	0.54	4.73	0.33	4.84	614	666
	-36°	<i>LCC</i>	0.53	4.19	0.33	5.11	594	559
	-55°	<i>LCC</i>	0.61	4.92	0.56	4.32	818	647
	$+36^\circ$	<i>LCC</i>	0.54	5.16	0.26	5.76	628	594
	$+55^\circ$	<i>LCC</i>	0.64	4.94	0.43	5.08	553	609
	0°	<i>PAI_e</i>	0.62	0.2	0.48	0.24	568	663
	-36°	<i>PAI_e</i>	0.64	0.22	0.48	0.26	772	601
	-55°	<i>PAI_e</i>	0.60	0.19	0.47	0.29	757	711
	$+36^\circ$	<i>PAI_e</i>	0.56	0.21	0.47	0.23	521	639
	$+55^\circ$	<i>PAI_e</i>	0.68	0.22	0.57	0.24	544	514
	0°	<i>CCC_e</i>	0.60	0.09	0.45	0.10	642	651
	-36°	<i>CCC_e</i>	0.56	0.10	0.45	0.12	772	559
	-55°	<i>CCC_e</i>	0.58	0.08	0.44	0.10	482	626
	$+36^\circ$	<i>CCC_e</i>	0.50	0.10	0.37	0.10	515	643
	$+55^\circ$	<i>CCC_e</i>	0.69	0.10	0.54	0.10	658	693
	0°	<i>All</i>	0.59	-	0.42	-	607	660
	-36°	<i>All</i>	0.57	-	0.42	-	718	574
	-55°	<i>All</i>	0.60	-	0.49	-	689	662
	$+36^\circ$	<i>All</i>	0.53	-	0.36	-	555	625
	$+55^\circ$	<i>All</i>	0.67	-	0.51	-	586	606

An examination of the cross-validated r^2_{cv} values for sequentially removed, least contributing bands for each of the GPR models shows that validation results generally remain stable as bands are removed from models (Figure 77, top left). Results were similar across all VZAs and vegetation variables: LCC was consistently the poorest, PAI_e was the best, and CCC_e was close to PAI_e. With respect to VZA, for LCC r^2_{cv} increased with fewer predictor variables and $+55^\circ$ and -55° showed the largest gains while $+36^\circ$ produced the poorest results as the number of variables decreased. In contrast, PAI_e r^2_{cv} was lowest at -55° , but produced some of the best results for $+55^\circ$. For CCC_e,

+55° was also the best when only a few predictor variables were included. It should be noted that these results differ from those of the ground based GPR assessment of Chapter 5, where +55° was among the worst performing VZAs and -55° the best. Overall, GPR models performed best with fewer than 10 predictor variables.

Figure 77 GPR model r^2_{cv} values for the vegetation variables and view angles. Graphs demonstrate modelling results as spectral features are removed from the optimized GPR model.

In a corresponding trend to the r^2_{cv} results, the associated cross-validated $RMSE_{cv}$ values for all vegetation variables showed an overall decrease as bands were eliminated from the models (Figure 78). However, in some instances $RMSE_{cv}$ jumped upwards when less than 5 predictor variables were left in the models; e.g., -36° for all vegetation variables. Also, nadir VZAs (0°) produced amongst the lowest $RMSE_{cv}$ values for each of the variables, even though r^2_{cv} values were not consistently the highest; this contrasts with the field scale analyses, which showed nadir view angle to be not a good as certain off-nadir angles for vegetation modelling and prediction.

Figure 78 Continuous $RMSE_{cv}$ values for the GPR models for various variables and look angles. Graphs demonstrate modelling error as spectral features are removed from the optimized GPR model.

The cross-validated GPR regression analysis results, when stratified by vegetation variable and VZA showed a high degree of variability. Overall, mean r^2_{cv} values were higher for PAI_e ($r^2_{cv}=0.62$, $RMSE_{cv}=0.21$) than for CCC_e ($r^2_{cv}=0.59$, $RMSE_{cv}=0.09$) or LCC ($r^2_{cv}=0.57$, $RMSE_{cv}=4.78$). Visualization of these results can be seen in Figure 79, top left. It is particularly surprising that just one (the optimal) predictor variable performs very well in predicting each of the vegetation variables at each VZA; however, overall results demonstrate that the use of just one predictor variable for biochemical and biophysical variable retrievals was not an optimal approach for estimating chlorophyll content (leaf or canopy) or canopy structural variables in the Arctic (e.g. mean $r^2_{cv}=0.59$ vs mean $r^2_{cv}=0.44$).

A breakdown of the results with respect to VZA is shown in Figure 79 (top right and bottom right). Combined results indicate that the $+55^\circ$ VZA was best overall (mean $r^2_{cv}=0.67$), while $+36^\circ$ was the poorest (mean $r^2_{cv}=0.53$).

Figure 79 GPR r^2_{cv} results for full model and for best single band GPR model. Results are stratified by location, look angle, and vegetation variable.

Similar regionally based results are reported here as compared to the SR and ROSAVI analysis; Banks Island (2012) produced the best results for all vegetation variables (Figure 79); however, the Richardson Mountains (2014) site was very comparable (mean r^2_{cv} =0.679 and 0.676, respectively). Possible reasons for this were discussed in Chapter 5 and include the large spatial

variation observed for LCC, PAI_e, and CCC_e values on Banks Island. The higher accuracy for the Richardson Mountains site may be due to statistical overfitting, as the number of predictor variables in the GPR model may have been high compared to the number of independent observations on the ground, especially for +55° where the field sample size was $n=14$. This is the reason why -55° was eliminated from the analysis; 10-fold cross-validated retrievals produced r^2_{cv} of ~0.99 with a sample size of $n=11$. However, the +55° model retained high accuracy when the number of GPR model predictor variables was decreased to less than the sample size, so it is uncertain if overfitting was a factor.

Table 40 shows the best contributing and top-ranking bands for all vegetation variables, VZAs, and geographic locations. The weighted mean for each variable's optimal spectral bands was calculated using the associated r^2_{cv} values to determine a more meaningful spectral centre. Overall, it was shown that selected bands were in the pigment absorption and red-edge spectral regions with LCC extending a bit into the NIR (LCC: 553-818 nm; PAI_e: 514-772 nm; CCC_e: 515-772 nm). Histograms of the GPR band selections can be seen in Figure 80 (best overall cross-validated band selection; i.e. the best predictor variable) and Figure 81 (overall highest-ranking cross-validated bands; i.e. most used bands selected across model iterations). The selection of sensitive bands showed a response at lower wavelengths (e.g. ~450 nm), and all vegetation variables elicit similar spectral responses (similar bands were chosen). As previously discussed in Chapter 5, the modelled band selections can be explained by mechanisms of variable covariation (Ollinger, 2011).

Figure 80 Histograms of best spectral bands (i.e. the best predictor variable) selected in GPR modelling for vegetation variables and view angles. Field sites have been combined.

Figure 81 Histograms of best overall bands (i.e. most used bands selected across model iterations) selected in the GPR modelling using all variables and VZAs. Field sites have been combined.

The best overall single band and the highest ranked weighted bands were graphed in relation to VZA (Figure 82). The weighted best single band selections showed a very slight spectral shift in relation to VZA as reported for the VI band selections, and once again differing from that obtained in the field-based assessment (Chapter 5).

Figure 82 GPR band selections by VZA for combined vegetation variables and individually for LCC, PAI_e, and CCC_e.

Scatter plots demonstrating various optimal cross-validated predictions (measured vs. predicted) are shown below for various field sites (LCC, Herschel Island -36°; PAI_e, Banks Island +55°; CCC_e; Richardson Mountains 2014 0°) (Figure 83). Variable over-prediction is apparent in each of the relationships. Because of the poor quality of the ARTMO GPR-BAT output maps (e.g. outputs did not contain spatial coordinates), cross-validated GPR modelled maps LCC, PAI_e, and CCC_e are not presented.

Figure 83 Scatterplots showing measured vs. predicted relationships for GPR modelling for various field sites and VZAs.

7.3.4. Physically based radiative transfer modelling: LMA inversion of PROSAIL

Figure 84 shows the performance of the LMA curve fitting procedure for various VZAs and field sites (inverted modelled parameters are shown for each curve) using the original parameter space (Table 33, Chapter 6). Figure 85 shows the performance of the LMA curve fitting procedure for various VZAs and field sites using the constrained parameter space (Table 36, Chapter 6). In these examples, the simulated directional-reflectance spectra were in good agreement with the measured TOC reflectance values ($r^2 \sim 0.99$, $RMSE = 0.005 \pm 0.005$) when using the original parameters; however, LMA inversions produced slightly less accurate fits with the constrained parameter space ($r^2 = 0.98-0.99$, $RMSE = 0.008 \pm 0.003$). Overall, the curve fitting algorithm, set to iterate 5000 times, was capable of reproducing TOC directional-reflectance for all value ranges of LCC, PAI_e, and CCC_e, (i.e. low to high values) and at all VZAs for both parameters sets. Neither the initial or constrained parameter values used for the analyses resulted in the algorithm getting stuck in local minima.

Figures 86 and 87 show the differences between the modelled (original parameter space and constrained parameter space, respectively) and measured reflectance values for the various sites and VZAs shown in Figures 84 and 85 (modelled values were subtracted from measured values to highlight over and under prediction of PROSAIL). Similar to the field-scale results reported in Chapter 6, the greatest observed error between the measured and modelled directional spectra occurred in the following spectral regions: (1) wavelengths less than ~500 nm (over prediction), (2) peak green reflectance centered at ~551 nm (over prediction), (3) pigment absorption centered at ~680 nm (under prediction), (4) wavelengths in the RE and NIR between ~700 nm to 750 nm (over prediction), (5) reflectance in the NIR centered at ~785 nm (under prediction), and (6) wavelengths greater than 990 nm (over prediction). Error patterns appear to be systematic (i.e. non-random) and observable for both the original parameter space and the constrained parameter space for all sites and VZAs. The TOC reflectance values in these spectral regions is either not well measured (especially in wavelength regions $<\sim 500$ nm and $>\sim 987$ nm), as was discussed earlier with respect to inherent noise associated with spectroradiometers (Chapters 5 and 6), or, more likely, not well modelled by the PROSAIL RTM (e.g. the parameter values may be off/incorrect or the PROSAIL model requires recalibration to match Arctic conditions). The observed spectral matching errors may also have been attributable to the following: (1) the CHRIS/PROBA ACM atmospheric correction may have produced erroneous surface reflectance values due to estimated (missing) metadata parameters (e.g. VZA, VAA, SZA, SAA, and RAA values) thus resulting in erroneous MODTRAN4 LUT inversion results, (2) the estimated VZA, VAA, SZA, SAA, and RAA values may have provided incorrect parameterization for PROSAIL, (3) the spatial averaging of the subplot field data into plot scale assumptions may have provided a source of error for the parameter space (i.e. averaged surrounding pixel values), and (4) assumed

value ranges for variables not measured at specific field sites (e.g. carotenoids) may not have been correct for sites outside of Richardson Mountains (2014).

Figure 84 Measured vs. modelled PROSAIL simulated TOC reflectance for various field sites and VZAs. Accompanying inverted PROSAIL leaf and canopy parameters are shown. Inversion results are for original inversion parameters.

Figure 85 Measured vs. modelled PROSAIL simulated TOC reflectance for various field sites and VZAs. Accompanying inverted PROSAIL leaf and canopy parameters are shown. Inversion results are for constrained inversion parameters.

Figure 86 Difference (Δ) between the modelled (using the original parameter space) and measured TOC spectral-directional reflectance values for full spectrum CHRIS/PROBA M1 datasets for various field locations and view zenith angles (VZA). Each plot shows all modelled spectra for that location and VZA.

Figure 87 Difference (Δ) between the modelled (using the constrained parameter space) and measured TOC spectral-directional reflectance values for full spectrum CHRIS/PROBA M1 datasets for various field locations and view zenith angles (VZA). Each plot shows all modelled spectra for that location and VZA.

The results for the LMA iterative numerical optimization inversion in terms of vegetation model quality are shown in Table 41. Correlation coefficient (r^2) values are presented using a red/white/blue colour ramp to highlight poor (blue, $r^2=0$) to median (white, $r^2=0.5$) to optimal results (red, $r^2=1$). Results are presented for both the original and constrained parameter spaces for all vegetation variables across all measurement scenarios (i.e. locations/angles). They demonstrate

that a larger parameter space (i.e. the original parameters) results in better model performance ($r^2=0.28$), as compared to using a constrained parameter space that was based on inverted field-scale spectra ($r^2=0.25$). Results were poorer than for the empirical modelling, but close to the field scale inversion results (Chapter 5; overall $r^2=0.33$), and RMSE values were correspondingly higher than those of the empirical modelling retrievals.

Table 41 PROSAIL modelling results for LMA inversion using the original and constrained inversion parameters. Plotted relationships are bolded and marked with an asterisk.

Colour Scale (r^2)		CHRIS/PROBA M1: LMA Inversion of PROSAIL				
			Original Parameters		Constrained Parameters	
Location	VZA	Variable	r^2	RMSE	r^2	RMSE
Herschel Island (2011)	0°	LCC	0.08	5.34	0.21	5.32
		PAI_e*	0.20	0.34	0.40	0.28
		CCC _e	0.36	0.13	0.23	0.12
	-36°	LCC	0.01	6.18	0.01	8.82
		PAI _e	0.09	0.39	0.18	0.27
		CCC _e	0.09	0.17	0.00	0.15
	-55°	LCC	0.08	5.18	0.01	7.34
		PAI _e	0.02	0.38	0.39	0.23
		CCC _e	0.01	0.14	0.23	0.11
	+36°	LCC	0.32	4.71	0.05	7.77
		PAI _e	0.04	0.41	0.19	0.25
		CCC _e	0.14	0.16	0.20	0.11
	+55°	LCC	0.17	5.86	0.00	7.43
		PAI _e	0.04	0.43	0.56	0.24
		CCC _e	0.41	0.12	0.18	0.12
Banks Island (2012)	0°	LCC	0.57	14.01	0.61	9.93
		PAI _e	0.48	0.64	0.65	0.63
		CCC _e	0.57	0.08	0.63	0.11
	-36°	LCC	0.46	16.05	0.60	13.30
		PAI _e	0.38	0.59	0.15	0.61
		CCC_e*	0.70	0.06	0.52	0.08
	-55°	LCC	0.48	12.73	0.64	10.14
		PAI _e	0.44	0.51	0.30	0.60
		CCC _e	0.45	0.07	0.43	0.10
	+36°	LCC	0.39	12.61	0.40	13.33
		PAI _e	0.07	0.66	0.09	0.62
		CCC _e	0.30	0.22	0.49	0.08
	+55°	LCC	0.56	9.64	0.30	11.66
		PAI _e	0.27	0.65	0.15	0.63
		CCC _e	0.49	0.14	0.32	0.13
Richardson Mountains (2013)	0°	LCC	0.37	6.09	0.35	5.90
		PAI _e	0.02	0.23	0.17	0.20
		CCC _e	0.58	0.08	0.32	0.10
	-36°	LCC	0.23	7.76	0.21	7.65

		PAI_e	0.05	0.25	0.20	0.17
		CCC_e	0.42	0.09	0.46	0.09
-55°	LCC		0.35	6.20	0.29	5.43
	PAI_e		0.24	0.18	0.29	0.19
	CCC_e		0.32	0.10	0.24	0.10
+36°	LCC^*		0.45	6.32	0.15	6.70
	PAI_e		0.19	0.21	0.30	0.20
	CCC_e		0.44	0.09	0.25	0.11
+55°	LCC		0.34	6.57	0.39	4.55
	PAI_e		0.31	0.17	0.17	0.19
	CCC_e		0.45	0.09	0.47	0.08
<i>Richardson Mountains (2014)</i> 0°	LCC		0.34	5.12	0.17	5.65
	PAI_e		0.02	0.38	0.04	0.37
	CCC_e		0.16	0.16	0.08	0.16
-36°	LCC		0.29	4.81	0.25	5.27
	PAI_e		0.52	0.38	0.32	0.36
	CCC_e		0.08	0.17	0.03	0.17
-55°	LCC		0.32	5.47	0.14	3.77
	PAI_e		0.15	0.37	0.02	0.39
	CCC_e		0.08	0.16	0.16	0.15
+36°	LCC		0.13	5.09	0.20	4.00
	PAI_e		0.52	0.30	0.01	0.39
	CCC_e		0.32	0.14	0.01	0.17
+55°	LCC		0.14	6.44	0.02	6.35
	PAI_e		0.20	0.33	0.15	0.33
	CCC_e		0.05	0.15	0.20	0.13
<i>All sites</i>	Overall		0.28	-	0.25	-
<i>All</i>	LCC		0.30	7.61	0.25	7.52
<i>All</i>	PAI_e		0.21	0.39	0.23	0.36
<i>All</i>	CCC_e		0.32	0.13	0.27	0.12
0°	LCC		0.34	7.64	0.34	6.70
-36°	LCC		0.25	8.70	0.27	8.76
-55°	LCC		0.31	7.40	0.27	6.67
+36°	LCC		0.32	7.18	0.20	7.95
+55°	LCC		0.30	7.13	0.18	7.50
0°	PAI_e		0.18	0.40	0.32	0.37
-36°	PAI_e		0.26	0.40	0.21	0.35
-55°	PAI_e		0.21	0.36	0.25	0.35
+36°	PAI_e		0.21	0.40	0.15	0.37
+55°	PAI_e		0.21	0.40	0.26	0.35
0°	CCC_e		0.42	0.11	0.32	0.12
-36°	CCC_e		0.32	0.12	0.25	0.12
-55°	CCC_e		0.22	0.12	0.27	0.11
+36°	CCC_e		0.30	0.15	0.24	0.12
+55°	CCC_e		0.35	0.13	0.29	0.12
0°	<i>All</i>		0.31	-	0.32	-
-36°	<i>All</i>		0.28	-	0.24	-
-55°	<i>All</i>		0.25	-	0.26	-
+36°	<i>All</i>		0.28	-	0.20	-
+55°	<i>All</i>		0.29	-	0.24	-

Visualization of the inversion results based on vegetation variable, parameter set, geographic location, and VZA can be seen in Figure 88. When results were stratified based on vegetation variable (top right), the PROSAIL unconstrained parameter set inversion produced overall higher mean r^2 values for CCC_e ($r^2=0.32$, RMSE=0.13) than for LCC ($r^2=0.30$, RMSE=7.61) or PAI_e ($r^2=0.21$, RMSE=0.39). A similar ranking was produced for constrained inversion; however, overall lower r^2 were produced for each of the vegetation variables while RMSE values improved slightly: CCC_e ($r^2=0.27$, RMSE=0.12), LCC ($r^2=0.25$, RMSE=7.52), and PAI_e ($r^2=0.23$, RMSE=0.36). Better LCC and poorer PAI_e models obtained here contrast with results obtained by other similar PROSAIL studies (e.g. Darvishzadeh et al., 2008a) that showed that leaf area and canopy chlorophyll content were better predicted than at the leaf scale. With respect to VZA, the strength of relationships for LCC, PAI_e, and CCC_e are highly variable in an almost random fashion (Figure 88, top right). It is possible that the PROSAIL model is not capable of effectively handling angular reflectance or ill-posedness of the inversion is not being accounted for.

Figure 88 PROSAIL results for original and constrained LMA inversion parameters. Results are stratified by location, look angle, and vegetation variable.

Stratifying by geographic location (Figure 88, lower left), similar results were obtained as for the empirical analysis. Banks Island (2012) produced the best overall correlations for all vegetation variables (e.g. For the constrained parameter set at 0° VZA: LCC, $r^2=0.61$, RMSE=9.93; PAI_e, $r^2=0.65$, RMSE=0.63; CCC_e, $r^2=0.63$, RMSE=0.11). As discussed previously in the thesis, the strong correlation results achieved in the Banks Island field site may be due to the larger spatial variation observed for LCC, PAI_e, and CCC_e values as compared to other field sites (i.e. greater differences in observed between min/max values and between field plots).

Stratification of inversion results based on VZA is shown in Figure 88 (bottom right). Nadir VZA (0°) produced the best overall results (original and constrained parameters $r^2=0.31$), followed by $+55^\circ$ for the original parameters ($r^2=0.29$), and -55° for the constrained parameters ($r^2=0.26$). These results are like the SR and ROSAVI modelling results of this chapter, where 0° produced the best correlation results; however, they differ from the GPR modelling, where best correlation

results were achieved at $+55^\circ$. Comparison of the CHRIS/PROBA inversion results to that of the field-based inversion results (Chapter 6) showed a similar pattern: the nadir VZA (0°) produced the best results ($r^2=0.44$) followed by $+55^\circ$ ($r^2=0.39$).

Scatter plots demonstrating PROSAIL inversions of the CHRIS dataset vs. measured field values are shown below (Figure 89) for various field sites and measurement scenarios (LCC, Richardson Mountains $+36^\circ$; PAI_e, Herschel Island 0° ; CCC_e, Banks Island -36°). Like the PROSAIL results of Chapter 6, LCC relationships appear to show negative bias, whereas PAI_e and CCC_e show varying degrees of positive bias.

Figure 89 Scatterplots showing measured vs. predicted relationships for original and constrained LMA PROSAIL inversions for various field sites and VZAs.

7.3.5. Summary of prediction results (SR, ROSAVI, GPR, and PROSAIL)

All results based on the $NRMSE_{cv}$ and $NRMSE$ are presented in Table 42 using a red/white/blue colour ramp to highlight poor (blue, $NRMSE_{cv}/NRMSE=0.40$) to median (white, $NRMSE_{cv}/NRMSE=0.20$) to optimal results (red, $NRMSE_{cv}/NRMSE=0.0$). When all vegetation variables (LCC, PAI_e, and CCC_e) and VZAs were averaged across field sites, it was shown that

the SR produced the best model accuracies ($\text{NRMSE}_{\text{cv}}=0.14$) followed by GPR (i.e. using the best modelling result) ($\text{NRMSE}_{\text{cv}}=0.16$), ROSAVI ($\text{NRMSE}_{\text{cv}}=0.17$), and the non-constrained LMA inversion of PROSAIL ($\text{NRMSE}=0.27$). These results contrast with the correlation based (r^2_{cv} and r^2) results (this Chapter), where GPR produced the top correlations ($r^2_{\text{cv}}=0.59$), followed by SR ($r^2_{\text{cv}}=0.53$), ROSAVI ($r^2_{\text{cv}}=0.48$), and PROSAIL ($r^2=0.28$). The overall results point towards optimal models being selected from iteration-based empirical approaches (i.e. SR and GPR).

Table 42 NRMSE_{cv} and NRMSE results for the empirical and physical modelling. Results calculated across field sites have been combined.

Colour Scale (NRMSE)			CHRIS/PROBA M1: Full Spectrum				All
			SR	ROSAVI	GPR	PROSAIL	All
Location	Angle	Variable	NRMSE_{cv}	NRMSE_{cv}	NRMSE_{cv}	NRMSE	NRMSE
<i>All</i>	<i>All</i>	<i>LCC</i>	0.13	0.16	0.15	0.25	0.17
	<i>All</i>	<i>PAI_e</i>	0.17	0.21	0.20	0.38	0.24
	<i>All</i>	<i>CCC_e</i>	0.11	0.14	0.13	0.18	0.14
	0°	<i>LCC</i>	0.12	0.14	0.15	0.24	0.16
	-36°	<i>LCC</i>	0.12	0.15	0.13	0.27	0.17
	-55°	<i>LCC</i>	0.15	0.18	0.14	0.24	0.18
	+36°	<i>LCC</i>	0.13	0.14	0.16	0.23	0.17
	+55°	<i>LCC</i>	0.12	0.17	0.15	0.24	0.17
	0°	<i>PAI_e</i>	0.16	0.20	0.19	0.39	0.24
	-36°	<i>PAI_e</i>	0.18	0.21	0.20	0.39	0.25
	-55°	<i>PAI_e</i>	0.18	0.20	0.20	0.35	0.23
	+36°	<i>PAI_e</i>	0.17	0.20	0.20	0.39	0.24
	+55°	<i>PAI_e</i>	0.18	0.21	0.21	0.39	0.25
	0°	<i>CCC_e</i>	0.11	0.14	0.12	0.16	0.13
	-36°	<i>CCC_e</i>	0.12	0.15	0.14	0.17	0.15
	-55°	<i>CCC_e</i>	0.09	0.12	0.11	0.16	0.12
	+36°	<i>CCC_e</i>	0.11	0.14	0.13	0.22	0.15
	+55°	<i>CCC_e</i>	0.12	0.14	0.14	0.18	0.15
	0°	<i>All</i>	0.13	0.16	0.15	0.26	0.18
	-36°	<i>All</i>	0.14	0.17	0.16	0.28	0.19
	-55°	<i>All</i>	0.14	0.16	0.15	0.25	0.18
	+36°	<i>All</i>	0.14	0.16	0.16	0.28	0.19
	+55°	<i>All</i>	0.14	0.18	0.17	0.27	0.19
	<i>All</i>	<i>All</i>	0.14	0.17	0.16	0.27	-

The vegetation variable that was best predicted across all sites was the CCC_e (mean value across all VZAs, datasets, and models; $\text{NRMSE}=0.14$), followed by LCC ($\text{NRMSE}=0.17$) and PAI_e ($\text{NRMSE}=0.24$). The superior prediction of CCC_e as compared to LCC follows the results of

Chapter 5 and 6 and similar empirical/physical retrieval studies (e.g. Darvishzadeh et al., 2008a); however, the relatively poor prediction of PAI_e in comparison to both CCC_e and LCC diverges from such studies (e.g. Curran et al., 1992; Baret & Jacquemoud et al., 1994; Darvishzadeh et al., 2008a). Reasons for this are discussed in previous Chapters (5 and 6) and points mainly towards poor signal propagation from leaf to canopy scales (e.g. Asner et al., 1998; Jacquemoud et al., 1996); theoretically, PAI_e should show better results than that of LCC. The combined mean prediction results showed that all VZAs produced rather similar $NRMSE_{cv}$ and NRMSE values (e.g. mean values for all combined datasets $NRMSE=0.19\pm0.01$), with 0° and -55° producing the best overall mean predictions ($NRMSE=0.18$). In contrast, results from the field-based approaches showed comparable results for most VZAs (i.e. 0° , -36° , $+55^\circ$, and -55°) for the empirical modelling (Chapter 5; mean $NRMSE_{cv}=0.15$), and the selection of 0° , -55° , and $+55^\circ$ for the physical modelling (Chapter 6; mean $NRMSE=0.29\pm0.01$). Finally, magnitude of the $NRMSE_{cv}$ and NRMSE values (when stratified according to modelling method) are like that of the field-based studies (Chapters 5 and 6) and suggest that the field-sampling approach (i.e. spatial averaging across the subplots) was appropriate for the spatial resolution of the CHRIS/PROBA sensor.

7.4. Discussion and Conclusions

In this study, a satellite-based, multi-angle, multi-method spectroscopic analysis of Arctic vegetation was conducted across a bioclimatic gradient in the Western Canadian Arctic between the years 2011 to 2014. To date there have been no studies using satellite-based imaging spectroscopy to retrieve biochemical or biophysical variables (i.e. LCC, PAI_e , or CCC_e) from Arctic tundra vegetation. Results demonstrate that scaled-up ground-based studies (Chapters 5 and 6) are effective at assessing/emulating the capabilities of spaceborne sensors. Overall results also

demonstrate the importance of methodological testing across multiple sites within large biomes/ecosystems. Key findings of this assessment are presented here with respect to the following: (1) multi-angle CHRIS/PROBA M1 spectral characterization of Arctic tundra; (2) performance of vegetation modelling and variable prediction using empirical approaches: a) a multi-band vegetation index (SR) with optimized spectral bands; b) a predefined soil-adjusted narrowband vegetation index (ROSAVI); c) a machine learning regression algorithm (GPR); and (3) performance of the PROSAIL RTM for simulating TOC reflectance of Arctic tundra and its subsequent inversion using LMA for retrieving the same vegetation variables.

7.4.1. Multi-angle CHRIS/PROBA M1 spectral characterization of Arctic tundra

Analysis of the multi-angle CHRIS/PROBA M1 TOC reflectance spectra revealed sun-target-sensor angular dependencies across all field sites. Backscatter VZAs (-55° and -36°) typically produced the greatest overall reflectance values, as expected due to (a probable) lack of shadows when the angular difference between the sensor and the sun is relatively small (forward scattering observations contain more signal from shaded leaves and branches) (e.g. Stagakis et al., 2010). Extracted nadir spectra typically produced the lowest reflectance across all sites and wavelengths, thus providing evidence that short vegetation tundra nadir measurements may be highly affected by canopy gaps (i.e. soils backgrounds and non-green vegetation components) and/or micro-shadows caused by hummocks (micro being in relation to the spatial resolution of the CHRIS/PROBA imagery ~ 34 m). It has been stated in previous multi-angle remote sensing research that canopy gap fractions typically decrease the quality and often the reflectance values of the signal, and may be most prevalent in nadir images (Deering et al., 1999; Sandmeier et al., 1998; Stagakis et al., 2010). However, there were several exceptions described below where the forward scatter reflectance spectra deviated from the expected values, and this may be due to the

low stature of the canopy, the presence of hummocks, the aspect/slope of the sampled plots, and/or the extreme sun-target-sensor angles (as most CHRIS/PROBA acquisitions were in the late afternoon).

(1) Herschel Island positive VZAs ($+36^\circ$ and $+55^\circ$) produced reflectance values that were slightly lower than the averaged nadir spectra. At this study site hummocks were prevalent across many of the field plots, therefore possibly contributing shadows at nadir and in the forward scatter VZAs. It is theorized that the low sun angle (66° SZA) in combination with greater degree of visible micro-shadows caused by hummocks may have contributed to larger visible shadowing within the positive VZAs thus causing a lower and similar reflectance shape to nadir observations. It is also possible that some of the field plots, as several were sampled on (gradual) slopes, were facing away from the sun/sensor (due to the extreme sun/sensor geometry encountered in the Arctic) thus producing an attenuation in the overall reflectance signal. It should be noted that all fieldwork was conducted during times where such aspects/slopes would not have had such a pronounced effect on spectral reflectance. Steep slopes were avoided during field sampling to reduce such slope related effects in the remote sensing analysis. Furthermore, the RAA of all three VZAs were within 8° of one another and VZAs were all greater than $+15^\circ$ thus adding to the similarity between signals. (2) The Richardson Mountains (2013) nadir and $+36^\circ$ VZA reflectance values were very similar. Reasons for this may be the similarity between the actual nadir observation angle and the $+36^\circ$ observation angle (e.g. $\sim 21^\circ$ vs. $\sim 40^\circ$), and the RAA of the nadir measurement being closer to the $< 60^\circ$ backscatter requirement ($\sim 98^\circ$ vs. $\sim 173^\circ$, respectively). (3) The Richardson Mountains (2014) $+55^\circ$ and -55° VZAs produced very similar surface reflectance values. Typically, backscatter reflectance is greater than forward scatter (as was observed at the field scale); however, in this instance both were of the same intensity. This was not likely due to

parameterization of the CHRIS/PROBA ACM as QUAC (which does not require parameterization) results showed the same angular response. Physical explanations may be that (a) less hummocky surfaces (flatter), and those imaged with higher sun angles, may exhibit typical volume scattering or a reflectance response that is more parabolic as one progresses from backscatter to forward scatter reflectance (e.g. Zhang et al., 2016), and (b) aspect and slope may have played a role due to the extreme sun/sensor angles within the mountains – although steps were taken to sample flat terrain. Finally, the Richardson Mountains NIR reflectance was greater in 2014 than in 2013 at all VZAs. Such differences may have been due to presence of higher quantities of leaf/canopy water in 2013, thereby attenuating the NIR signal, or a more advanced phenological stage in 2014 resulting in increased NIR reflectance as the image dates were July 6 and August 2, respectively.

CHRIS/PROBA spectra extracted across all field sites and all VZAs did not possess standard/typical vegetation curves. Instead, TOC vegetation reflectance values followed the same curves as reported in the field based spectral analysis (Chapter 5) and in similar field-based studies (e.g. Buchhorn et al., 2013; Bratsch et al., 2016; Liu et al., 2017). As discussed previously in Chapter 5, the visible soils/substrates (i.e. gap fractions), variability of the photosynthetic vegetation components (i.e. pigment pools), and non-photosynthetic vegetation components (i.e. senescent vegetation/structural components) are assumed to heavily influence reflectance and absorption across the VIS, RE, and NIR regions causing a general progressive increase/curve. Like the variability of the ground-based spectra, the greatest variability in the CHRIS/PROBA reflectance signals appeared in the VIS/RE regions, specifically in all regions below ~530 nm and in regions between ~600-700 nm (with peak variability at ~680 nm, i.e. chlorophyll absorption). Reasons for the observed variability have been previously discussed (Chapter 5) and may relate to

such phenomena as sensor noise (especially at ~442 nm), and spatial variability of gap fractions, pigment pools, and leaf/canopy structure. Finally, like the ground spectra, the CHRIS/PROBA spectra showed no observable and consistent patterns related to variability across the various VZAs and field sites.

7.4.2. Empirical modelling retrievals

7.4.2.1. Simple ratio vegetation index (SR)

The SR VI approach was shown to produce the second-best correlation-based results and the best prediction-based results when tested with the multi-angle CHRIS/PROBA M1 imagery (mean $r^2_{cv}=0.53$, $\text{NRMSE}_{cv}=0.14$). These results were very similar to but only slightly better than the field-based SR assessment (mean $r^2_{cv}=0.51$, $\text{NRMSE}_{cv}=0.15$). Conclusions drawn from the CHRIS/PROBA SR analysis are as follows.

(1) Overall, it was shown that PAI_e produced the best correlation-based results from the multi-angle reflectance spectra at all field sites and across all VZAs ($r^2_{cv}=0.59$), followed by CCC_e ($r^2_{cv}=0.55$). LCC had the poorest correlation-based results ($r^2_{cv}=0.45$). It is not surprising that PAI_e and CCC_e produced similar results to one another and better overall results than LCC. PAI_e and CCC_e were highly correlated across all study sites (mean $r^2=\sim 0.88$), whereas LCC values remained relatively uniform across all plots and field sites and had lower correlations to PAI_e (mean $r^2=\sim 0.24$). It is possible that LCC is difficult to estimate from the spectral reflectance because of the high species diversity (i.e. high variability of chlorophyll quantities based on plant type; see Chapter 3) and vertical gradients of chlorophyll content within the structure of the canopy (e.g. shaded leaves likely possess different quantities of chlorophyll than sun lit leaves, etc.). As previously stated in Chapters 5 and 6, reflectance-based studies typically point towards poor signal propagation from leaf to canopy and accordingly conclude that canopy scale variables are

characteristically easier to estimate (Asner, 1998; Jacquemoud et al., 1996; Yoder & Pettigrew-Crosby, 1995). However, in contrast, model predictions/accuracies showed that CCC_e produced the best results ($NRMSE_{cv}=0.11$), followed by LCC ($NRMSE_{cv}=0.13$), then PAI_e ($NRMSE_{cv}=0.17$). Similar results were obtained in the field-based SR VI assessment (Chapter 5) and have been obtained in similar empirical studies (i.e. CCC produces better overall accuracies than LCC) (e.g. Darvishzadeh et al., 2008a), but differ from studies that show LAI is easier to predict than LCC (Darvishzadeh et al., 2008a; Atzberger et al., 2015). The poor estimation of PAI_e is likely related to the low stature and complexity of Arctic canopies (i.e. number of species present, species morphology, etc.) and/or the presence/absence of gap fractions/non-photosynthetic vegetation components.

(2) The band optimization analysis using the SR aimed to reveal the wavelength regions of the multi-angle reflectance signals and their potential for estimating the biochemical and biophysical vegetation variables. The optimal wavelengths selected were shown to be highly variable across VZAs and field sites; however, optimal wavelength regions were somewhat in-line with well-known spectral absorption regions for pigments (i.e. LCC, PAI_e , and CCC_e) in the VIS (e.g. ~519-756 nm) and their associated structural components (i.e. cell and canopy structure) in the RE and NIR regions (e.g. ~576-847 nm), as reported in the field-scale analysis (Chapter 5) and in previous studies examining green vegetation components (e.g. Buchhorn et al., 2013; Bratsch et al., 2016; Liu et al., 2017). However, the selection of bands outside of those wavelength regions also occurred for all variables. For example, LCC showed band selections as low as 442 nm and as high as 976 nm with optimal bands selections for B1 of 539-681 nm and B2 of 702-847 nm; PAI_e showed band selections in the low 500 nm range up to 997 nm with optimal wavelengths with optimal band selections for B1 of 627-711 nm and for B2 of 626-678 nm; and CCC_e showed band

selections from 500 nm to 976 nm with optimal selections for B1 of 519-756 nm and for B2 of 576-738 nm. The selection of similar bands between variables and outside of known ranges can be explained by mechanisms of variable covariation (as previously discussed in Chapters 5 and 6) (Ollinger, 2011; Stagakis et al., 2010; Verrelst et al., 2016). Furthermore, the selection of bands outside of the expected ranges have been known to appear by chance or through indirect reflectance responses to biochemical constituents, canopy structural, and non-vegetated background components (Stagakis et al., 2010; Haboudane et al., 2004; Filella & Peñuelas, 1994). In this research, it is possible that gaps within the canopy (i.e. exposed non-green vegetation and non-vegetation materials) are driving wavelength selections outside of expected ranges.

(3) A very slight spectral shift was detected for all vegetation variables with respect to VZA. It was shown that weighted selection of optimal bands decreased in wavelength as VZAs progress from backscatter to forward scatter. This disagreed with the field-scale analysis that showed the opposite trend. To further explore this phenomenon, there should be a more in-depth analysis at the field scale. The conditions under which field measurements were taken (e.g. sun-target-sensor geometry, direct/diffuse lighting) differed from those of the CHRIS/PROBA satellite acquisitions. Furthermore, the field measurements were integrated over various sun positions as opposed to the sun position being almost constant for the CHRIS/PROBA acquisition. Explanations for the shift in wavelength were previously attempted (Chapter 5), but may not hold up in this scenario. Further, it is possible that the ground based spectral assessment is not capturing the true reflectance behavior as compared to the satellite based spectral measurements (dependent on scale of observation).

(4) The VZA that produced the optimal results with SR was nadir (0°) ($r^2_{cv}=0.56$, $\text{NRMSE}_{cv}=0.13$) followed by forward scatter VZAs ($+55^\circ$ $r^2_{cv}=0.55$, $\text{NRMSE}_{cv}=0.14$; and $+36^\circ$

$r^2_{cv}=0.54$, $NRMSE_{cv}=0.14$). This differs from the ground-based analysis that produced the best overall results for extreme backscatter (-55°). As previously stated in the thesis (Chapters 5 and 6), studies examining the effect of view angle on the estimation of biochemical and biophysical variables have concluded that off-nadir observations can be more useful, since less background (i.e. smaller gap fractions) and shadows (i.e. when using backscatter observations) are visible within the IFOV (Takebe et al., 1990; Walter-Shea et al., 1997; Galvão et al., 2009). Indeed, other multi-angle studies have concluded that shadowing is not the driving factor regarding the reliability of the reflectance signal (i.e. lower importance), but instead the proportion of photosynthetic, non-photosynthetic and background compounds is important (Stagakis et al., 2010; Verrelst et al., 2008). This explanation may hold true in Arctic environments as shadowing is minimal compared to the degree of exposed soils/backgrounds (i.e. gap fractions) and non-photosynthetic materials (e.g. lichens and woody materials, etc.); however, the variability of the results based on VZA (between studies/methods) show no defined pattern or trend (i.e. due to the low stature of the canopy gap fractions would always be visible). Furthermore, multi-angle prediction (i.e. model accuracy) results were all very similar ($NRMSE_{cv}=0.135\pm0.01$) and point towards no distinct advantage between VZAs.

(5) Possible errors in the SR analysis (and the other modelling scenarios) may stem from, and might not be limited to, the following two sources: (a) the atmospheric correction of the CHRIS/PROBA data was based on estimated metadata values (e.g. VZA and VAA) and inverted atmospheric parameters (MODIS AOT and CWV values produced unacceptable surface reflectance values); and (b) the difference between field work measurements and the satellite acquisition dates (e.g. Richardson Mountains 2014).

7.4.2.2. Revised optimized soil adjusted vegetation index (ROSAVI)

The ROSAVI approach was shown to produce the third best retrieval results when tested with the multi-angle CHRIS/PROBA M1 imagery (mean $r^2_{cv}=0.48$, $NRMSE_{cv}=0.17$), and produced results that were similar but slightly worse than the ROSAVI field-based assessment (mean $r^2_{cv}=0.45$, $NRMSE_{cv}=0.18$). Conclusions drawn from the ROSAVI analysis are as follows.

(1) Like the SR results, ROSAVI produced the best correlation-based results for PAI_e ($r^2_{cv}=0.53$) followed by CCC_e ($r^2_{cv}=0.48$) then LCC ($r^2_{cv}=0.43$). As discussed, optimal correlation-based results for PAI_e/CCC_e may be due to the detectability of canopy structure versus that of leaf based biochemical composition. However, optimal prediction results contrasted with correlation-based results, and showed that CCC_e was best predicted ($NRMSE_{cv}=0.14$), followed by LCC ($NRMSE_{cv}=0.16$) then PAI_e ($NRMSE_{cv}=0.21$). Implications of this have been previously discussed.

(2) Wavelengths used in ROSAVI (703 and 748) are within the realm of meaningful spectral bands selected in the multi-band SR analysis; however, the wavelength positions used in combination with ROSAVI were deemed to be not optimal as is evident from the poorer results of the analysis. It is possible that the ROSAVI formulation explored through a multi-band optimization analysis as was conducted for SR has the potential to outcompete SR due to its ability to minimize background effects (i.e. non-photosynthetic materials and soils). Aside from this, the benefit of using fixed wavelengths in a predefined VI is that the universality of the formulation and the wavelength positions can be explored across measurement scenarios (i.e. geographic locations and VZAs), as opposed to the reselection of optimal bands for each image condition as was done with the multi-band approach in this research. The good agreement between the field-

based results and the remote sensing results point towards the suitability of the ground-based approach.

(3) The ROSAVI index was designed and tested to minimize background effects when predicting/retrieving vegetation biochemical and biophysical variables (Wu et al., 2008) and has not been used in Arctic environments. In this study, it was shown to perform better at nadir and positive VZAs than at backscatter VZAs, thus providing some evidence that such a soil-adjusted index may be working as intended within Arctic environments and may provide added benefit over traditional VIs when a greater degree canopy gaps and shadowing are visible (e.g. at nadir and forward scatter angles).

(4) Finally, it was shown that the optimal VZA used with ROSAVI for modelling all vegetation variables across all sites was 0° ($r^2_{cv}=0.54$, $\text{NRMSE}_{cv}=0.16$) followed by $+55^\circ$ ($r^2_{cv}=0.52$, $\text{NRMSE}_{cv}=0.18$), which aligned with the SR analysis but differed from the empirical field-based ROSAVI assessment. Multi-angle prediction (i.e. accuracy) results were all very similar ($\text{NRMSE}_{cv}=0.17\pm0.01$) and point towards no distinct advantage between VZAs.

7.4.2.3. Gaussian processes regression (GPR)

The GPR approach was shown to produce the best modelling results using multi-angle CHRIS/PROBA M1 imagery (mean $r^2_{cv}=0.59$) and second-best model accuracies ($\text{NRMSE}_{cv}=0.16$), and the results were only slightly lower than the GPR field-based assessment (mean $r^2_{cv}=0.61$, $\text{NRMSE}_{cv}=0.16$). Full spectrum methods have seldom been used for biophysical or biochemical retrievals in Arctic environments and additionally have not been tested for spectroscopic retrievals of LCC, PAI_e, or CCC_e from multi-angle imaging spectroscopy data. Conclusions drawn from the GPR analysis are as follows.

(1) Like the VI analyses, it was shown that the prediction of PAI_e was most easily implemented from the multi-angle reflectance spectra at all field sites and across all VZAs ($r^2_{cv}=0.62$), followed by CCC_e ($r^2_{cv}=0.59$). LCC had the lowest modelling results out of all the variables ($r^2_{cv}=0.57$). Like all previous analyses, CCC_e was best predicted ($NRMSE_{cv}=0.13$), followed by LCC ($NRMSE_{cv}=0.15$) then PAI_e ($NRMSE_{cv}=0.20$). Implications of this have been previously discussed.

(2) For each of the vegetation variables, spectral bands within the chlorophyll absorption region (~680 nm) and the red-edge reflectance regions (~720-820 nm) were found to be crucial for retrievals. In these regions, both pigment concentrations and vegetation structural attributes influence TOC reflectance. The importance of these regions has been demonstrated in other Arctic based studies (e.g. Buchhorn et al., 2013; Bratsch et al., 2016; Liu et al., 2017) and in the field-based assessment (Chapter 5). Accordingly, GPR results demonstrate that band selections are physically meaningful at all VZAs and across geographic locations. As stated before, the selection of bands outside of the expected ranges was encountered (i.e. variable covariation) (Darvishzadeh et al., 2008a; Stagakis et al., 2010; Verrelst et al., 2016).

(3) The use of one predictor variable (i.e. the optimal band) in the GPR model produced results that were comparable to ROSAVI, indicating that, while variable reduction is important, reducing to only one predictor will also degrade model quality. Optimal results were achieved when predictor variables were greater than 1 but less than 20. Darvishzadeh (2008a) also showed that variable retrievals in vegetation studies using partial least squares regression can benefit from cautiously selected spectral subsets.

(4) The spectral shift that was detected in the multi-band SR analysis was also detectable in the GPR band analysis. A decrease in optimal wavelength regions (averaged across all variables) was

detectable when progressing from negative to positive VZAs (i.e. backscatter to forward scatter). This result counters the results obtained at the field-scale analysis that showed the opposite trend. The differing results indicate that further analysis is required. All attempts were made in the field to measure reflectance as it is measured by the CHRIS/PROBA sensor; however, differences existed between the on-ground measures and the unpredictable CHRIS/PROBA acquisition angles.

(5) Finally, it was shown that the optimal VZA for modelling/predicting all vegetation variables across all sites was $+55^\circ$ ($r^2_{cv}=0.67$, $\text{NRMSE}_{cv}=0.17$), followed by -55° ($r^2_{cv}=0.60$, $\text{NRMSE}_{cv}=0.15$) and 0° ($r^2_{cv}=0.59$, $\text{NRMSE}_{cv}=0.15$) when using GPR. These results loosely aligned with the VI analysis but differed from the empirical field-based GPR assessment, where -55° was selected as the best VZA. Once again, multi-angle prediction (i.e. accuracy) results were all very similar ($\text{NRMSE}_{cv}=0.16\pm0.01$) and point towards no distinct advantage for any one VZA.

7.4.3. Physical modelling retrievals: LMA inversion of PROSAIL

The LMA based numerical inversion of PROSAIL was shown to produce the least accurate retrieval results when tested with the multi-angle CHRIS/PROBA M1 imagery (mean $r^2=0.28$, $\text{NRMSE}=0.27$). Results were very similar but slightly worse than the field-based PROSAIL inversion results (mean $r^2=0.33$, $\text{NRMSE}=0.32$). Conclusions drawn from the LMA based numerical inversion of PROSAIL are as follows.

(1) Overall, it was shown that CCC_e was the most easily predicted vegetation variable (mean $r^2=0.32$, $\text{NRMSE}=0.18$). As previously discussed, this may be attributable to the information content that exists within LCC and PAI_e when combined: they are known to conjointly control canopy reflectance (Darvishzadeh et al., 2008a; Stagakis et al., 2010; Olliger, 2011; Verrelst et al., 2016). Further, the enhanced retrieval of CCC_e agrees with the previous ground-based physical

modelling investigation and with similar remote sensing based PROSAIL retrieval studies (e.g. Darvishzadeh et al., 2008a). However, the LCC and PAI_e inversion results do not concur with the results of the empirical investigation. In most measurement scenarios (e.g. VZAs, field sites), PROSAIL produced superior correlation-based results for LCC ($r^2=0.30$) than for PAI_e ($r^2=0.21$), whereas the opposite occurred for the empirical retrievals.

Regarding the physical retrievals, it is possible that the PROSAIL model is not adequately simulating reflectance across multiple wavelength regions, as was shown in the modelled-measured relative error analysis. The largest TOC reflectance errors were detected across wavelength regions known to be sensitive to leaf biochemistry and leaf/canopy structure in Arctic vegetation canopies (e.g. see Chapter 5) (Buchhorn et al., 2013; Liu et al., 2017). It is also possible that due to variable covariation and the selection of important wavelengths in the lower wavelength regions (i.e. <530 nm), as shown in the GPR and multi-band SR VI assessment, the PROSAIL model might be further incapable of accurately simulating these wavelength regions. These errors may be attributable to the amount of noise encountered in the CHRIS/PROBA spectra or through improper calibration of the PROSAIL RTM for use in Arctic ecosystems; the observed systematic error patterns point towards model calibration issues. Furthermore, it is also possible that TOC reflectance is not being accurately modelled with respect to sun-target-sensor geometry since the results, stratified per vegetation variable and VZA, are quite variable. If the physical model is indeed generalizable across measurement scenarios, then lower variability would be expected. Although LCC produced superior results to PAI_e , it should be stated that the relationships between measured and estimated LCC were poor in all inversion scenarios when averaged across the bioclimatic gradient. These results align with studies that have shown difficulties in estimating LCC with PROSAIL in heterogeneous plant assemblages (Baret & Jacquemoud, 1994; Curran et

al., 1992; Darvishzadeh et al., 2008a), but differ from studies that show canopy variables (i.e. LAI) is easier to predict than leaf-based variables (i.e. LCC) (e.g. Darvishzadeh et al., 2008a).

(2) The overall poor results of the inversions may be explained by the inability of the one-dimension PROSAIL turbid medium model to accurately describe the radiation field of a complex heterogeneous canopy (e.g., gap fractions, clumping effects, multiple leaf layers having different optical characteristics, etc.). As described in Chapter 6, if the physical modelling assumptions are violated, it is expected that the PROSAIL model will fail outright (Meroni et al., 2004; Darvishzadeh et al., 2008a); in such an instance, alternative modelling assumptions should be considered (e.g. Verhoef & Bach, 2007). It has been shown by Darvishzadeh et al. (2008a) that short, heterogeneous grassland canopies can be simulated with PROSAIL at the remote sensing level; however, their results showed that the stratification of plant heterogeneity must be completed to increase accuracy. This suggests that PROSAIL is not well suited to naturally complex/heterogeneous multi-species Arctic tundra canopies.

In this study, and like the field-based study (Chapter 6), the Banks Island field site showed the best correlation-based results compared to the other field sites, but showed the highest error. These results, like those at the field-scale, demonstrate the importance of testing across multiple geographic locations within an ecosystem to fully assess the generalizability of the physical modelling approach.

(4) This study tested the directional capabilities of the PROSAIL model. Results showed that the model produced the best correlation based results at 0° ($r^2=0.31$, NRMSE=0.26) followed by $+55^\circ$ ($r^2=0.29$, NRMSE=0.27). Best model predictions were achieved at -55° ($r^2=0.25$, NRMSE=0.25). As reported in the field-based analysis of PROSAIL (Chapter 6), the variation in results across the different view angles establishes three possible uncertainties: (a) the model is

not fully capable of accounting for directional reflectance; (b) the inversion approach is not accounting for the ill-posed problems associated with RTMs (i.e. multiple solutions may exist to the model inversion); (c) the model is not being parameterized correctly due to the need for the estimation of CHRIS/PROBA angular parameters (e.g. VZA, VAA, and RAA). Once again, multi-angle prediction (i.e. accuracy) results were all very similar ($\text{NRMSE}_{\text{cv}}=0.27\pm0.02$) and point towards no distinct advantage for any one VZA.

(5) The LMA iterative numerical optimization inversion technique has not been extensively tested with the PROSAIL RTM (e.g. Hilker et al., 2017) or with the CHRIS/PROBA sensor, and has never been tested in Arctic tundra ecosystems to retrieve vegetation biochemical and biophysical parameters and variables from TOC multi-angle spectral reflectance. In this study, it was shown that the algorithm is capable of iterating the PROSAIL leaf and canopy parameter space to accurately simulate Arctic tundra TOC spectral reflectance across multiple field sites and varying sun-target-sensor geometries using CHRIS/PROBA data; however, the overall results of the parameter/variable inversions were generally poor. Considerations regarding the implementation of the LMA inversion strategy have been previously discussed in Chapter 6.

Regularization strategies (e.g. Combal et al. 2003; Meroni et al. 2004; Rivera et al., 2013) as implemented in this study showed that the reduction of the parameter space using the ground based inversion results (i.e. one standard deviation above and below the mean of the inverted results for unknown leaf and canopy parameters) and using the mean of all inverted parameters as starting values did not produce better r^2 values, but the NRMSE values did improve very slightly. The parameterization approach accounted for known variables (sun-target-sensor geometry) and known variable ranges (i.e. zero values where vegetation was known to be sparse/absent). It is possible that either some wavelengths are poorly measured (i.e. too much noise/instrument error)

or the model is not adequately simulating the TOC spectral reflectance by means of the chosen parameter space; however, as previously discussed (Chapter 6), the expansion of the parameter space (e.g. upper and lower boundaries of the parameters) does not necessarily lead to the amelioration of results and in the case of numerical optimization as used in this study, greatly increases the inversion time. Poor results encountered in this study may be also due to ill-posedness of the physical modelling approach.

7.4.4. Overall conclusions

Overall conclusions drawn from this study are as follows. (1) The remote sensing modelling results produced very similar results to the field-based modelling approaches (Chapters 5 and 6), thus providing confirmation that the spatial sampling methodology employed at the field scale was appropriate for scaling to the remote sensing level. (2) Iteration-based empirical modelling methodologies (i.e. SR and GPR) produced the best overall modelling results. Like the field-based approach, optimal weighted multi-angle spectral regions for variable retrievals (LCC, PAI_e, and CCC_e) were revealed to be largely within expected wavelength regions (e.g. extending from peak green reflectance at ~550 nm to RE/NIR reflectance at ~750 nm); however, due to the large degree of variable covariation observed in the band selections across all VZAs, future remote sensing studies should not discard wavelengths outside of this range (e.g. outside of known pigment absorption wavelengths). (3) The non-iterative empirical approach based on preselected wavelengths used in a soil-based VI (i.e. ROSAVI) was shown to produce the least accurate fits/model predictions; however, results were not substantially different from SR and GPR. Further investigation into the use of soil-based VIs is warranted due to the prevalence of gap fractions and non-photosynthetic materials in Arctic tundra canopies. (4) As expected, the PROSAIL model did not produce accurate inversion results, but did produce very similar results to the field-scale

inversions. The similarity between the field and remote sensing results provides some indication that PROSAIL is capable of being scaled to the remote sensing level in the Arctic. Further restriction of the PROSAIL parameter space using field-scale inverted values (i.e. regularization) did not result in improved inversion results. Analysis of the error patterns for the simulated TOC reflectance showed a systematic error pattern across field sites and VZAs. Implications of these results are: (a) it is likely that Arctic tundra canopies violate the assumptions behind the physical model, and (b) model calibration (e.g. refractive index and absorption coefficients of leaf constituents) should be explored for Arctic plants/canopies. Future research should consider examining additional RTMs and inversion methods.

Part III: Synthesis and Conclusions

Chapter 8. Synthesis and Conclusions

8.1. Introduction

The five studies (Chapters 3-7) of this thesis are summarized and brought together in this final synthesis chapter. In addition, statistical analyses of the combined field and remote sensing modelling results are presented (Section 8.5). All previous empirically-based tests were conducted using a k -fold cross-validation procedure (e.g. r^2_{cv} and NRMSE_{cv} as in Chapters 5 and 7), whereas all physically-based tests were not (e.g. r^2 and NRMSE as in Chapters 6 and 7). For simplicity, all results below are presented with the simplified notation (e.g. r^2 and NRMSE).

Overall, the goal of this research was to determine the capability and applicability of both empirical and physical modelling methodologies for retrieving leaf and canopy biochemical and biophysical characteristics of Arctic tundra vegetation from multi-angle, space-borne imaging spectroscopy data. To complete this goal, three levels of investigation were undertaken using field and remote sensing data from six field sites sampled across a bioclimatic (i.e. latitudinal) gradient representative of the variety of Arctic vegetation conditions in the Western Canadian Arctic.

- (1) A laboratory and field-based plant and canopy level investigation provided information on the biochemical (e.g. leaf and canopy chlorophyll content, LCC and CCC respectively) and biophysical (e.g. plant area index, PAI) characteristics of Arctic tundra vegetation across the bioclimatic gradient. The quantitative characterization and measurement of leaf biochemistry and canopy architecture was necessary for subsequent calibration and validation of optically-based empirical retrievals and physical model parameterization and validation.

- (2) Field-based multi-angle spectral measurements and subsequent modelling were investigated to provide insight into:
- i. scaling subplot ($\sim 1 \text{ m}^2$) measurements and retrievals to the plot scale (both spectral and biochemical/biophysical);
 - ii. the benefits of using full spectral narrowband information versus a resampled spectral subset derived to simulate spaceborne CHRIS/PROBA bands;
 - iii. the best approaches for empirical vegetation modelling, including:
 - a. the best multi-band vegetation index (VI) and the optimal bands to be applied in VI modelling using multi-angle spectral data;
 - b. the best predefined VI for the same multi-angle vegetation modelling purposes; and
 - c. the utility of a machine learning regression algorithm (i.e. Gaussian processes regression, GPR) for such vegetation modelling;
 - iv. the capability of a one-dimensional turbid medium leaf and canopy radiative transfer model (RTM) (i.e. PROSAIL) for simulating tundra top of canopy (TOC) reflectance spectra; and
 - v. the use of an iterative numerical optimization inversion method (Levenberg Marquardt algorithm, LMA) for inverting the PROSAIL model to predict measured leaf and canopy parameters/variables.
- (3) Insights from the field scale studies were applied in a remote sensing scale investigation for retrieving biochemical and biophysical variables from the empirical and physical models as described under (2) iii-v above. Such insights included: choice of optimal multi-band (i.e. simple ratio, SR) and predefined narrow band VIs (i.e. revised optimized soil adjusted

vegetation index, ROSAVI); the use of a spectral subset to improve the predictive accuracy of the GPR modelling; and insight into regularization strategies for use with PROSAIL (e.g. parameter start values, parameter space size, fixing variables, and model iterations).

8.2. Leaf and Canopy: Measurement and Latitudinal Characterization

A literature review identified that there is currently a lack of quantitative, field-measured information pertaining to leaf and canopy biochemical (e.g. chlorophyll, carotenoids, and water) and biophysical/structural (e.g. average leaf angle, average leaf weight, canopy gap fractions, and leaf/canopy clumping) characteristics of tundra vegetation as it exists across bioclimatic gradients in the Arctic. Studies examining the pigment biochemical aspects of tundra vegetation are rare (e.g. Tiezen & Johnson, 1968; Tiezen, 1970; Tiezen, 1972); those examining the spatial patterns of vegetation biochemistry across Arctic latitudinal/bioclimatic gradients are nonexistent. In contrast, many studies have measured and reported on Arctic tundra canopy structural components (e.g. leaf area index, LAI) and biomass/phytomass quantities that occur across various Arctic geographical transects (e.g. Epstein et al., 2008; Walker et al., 2008; Walker et al., 2011; Epstein et al., 2012; Raynolds et al., 2012; Walker et al., 2012; Walker et al., 2016). Therefore, the laboratory and field-based studies in this research (see 8.1 (1) above) were undertaken to provide such quantitative leaf and canopy information and to provide reference and calibration/validation data for the subsequent modelling efforts (e.g. leaf and canopy biochemical and biophysical data were necessary for the PROSAIL parameterization). Furthermore, at the time of commencing this research, the quantitative modelling and estimation of PAI using downward hemispherical photography (DHP) had not been previously reported in the literature and thus represented a unique aspect of this research.

8.2.1. Leaf/canopy biochemistry: Destructive and non-destructive measurements

The main findings of the leaf and canopy biochemical analysis (Chapter 3) were as follows.

(1) The results showed that the chlorophyll concentrations of dominant Arctic tundra species, if those species can be considered representative of other locations and species, typically average between $10.5 \mu\text{g}/\text{cm}^2$ to $57.2 \mu\text{g}/\text{cm}^2$ and possess an overall average of approximately $37.5 \mu\text{g}/\text{cm}^2$, inclusive of all species. Values did not differ substantially from the mean value of $38.0 \mu\text{g}/\text{cm}^2$ that was previously reported by Tiezen and Johnson (1968); however, the range (min/max) of values reported here were quite different. The values reported here were derived using updated and accepted extinction coefficients (Lichtenthaler, 1987).

(2) Field-based instrumental measurements demonstrated a latitudinal gradient of leaf and canopy chlorophyll content, from higher LCC at lower latitudes (e.g. $\sim 40.7 \mu\text{g}/\text{cm}^2$) to lower LCC at higher latitudes (e.g. $\sim 32.0 \mu\text{g}/\text{cm}^2$). Similarly, CCC showed a latitudinal gradient, with $0.45 \text{ g}/\text{m}^2$, $0.26 \text{ g}/\text{m}^2$, and $0.18 \text{ g}/\text{m}^2$ at low, medium and high latitudes, respectively. Latitudinal values of field-measured Arctic tundra LCC and CCC have not been previously reported in the literature, thus the regional characterization of leaf and canopy biochemistry represented a unique aspect of this research.

(3) The destructive lab/field-based chlorophyll measurements showed no statistical difference ($p < 0.05$) to plot-scale handheld chlorophyll measurements when converted using a consensus equation (Cerovic et al., 2012), thus indicating the potential for the generalized use of instruments for ground sampling in the Arctic (i.e. both the Minolta SPAD-502 and the linear consensus equation). Use of such handheld chlorophyll meters in the Arctic has not previously been presented in the literature.

(4) The characterization of leaf carotenoids and equivalent water thickness (EWT) has not been previously reported for the regions studied in this research. The results showed that carotenoid concentrations of the dominant Arctic tundra species range from $3.3 \mu\text{g}/\text{cm}^2$ to $23.0 \mu\text{g}/\text{cm}^2$ with average total values of approximately $14.6 \mu\text{g}/\text{cm}^2$, inclusive of all species. Lastly, EWT values range from approximately $0.01 \mu\text{g}/\text{cm}^2$ to $0.04 \mu\text{g}/\text{cm}^2$ with average values of $0.03 \mu\text{g}/\text{cm}^2$. Although, not the primary focus of the modelling retrievals in this research, derivation of such values (i.e. carotenoids and EWT) was considered important for parameterization of the physical modelling approach.

Subsequent vegetation-based biochemical research conducted in the Arctic should focus on comprehensive characterization of pigment (e.g. chlorophyll, carotenoids, and anthocyanins) and non-pigment (e.g. nitrogen, cellulose, lignin, and water) vegetation biochemistry across species, seasons, and representative environments (recognizing that multiple environments are difficult to access). Not only would such a dataset serve as baseline/reference data for retrieval studies, but would allow for further refinement of RTMs that are increasingly incorporating additional leaf/canopy parameters into their code (e.g. PROSPECT-D) (Feret et al., 2017).

8.2.2. Canopy structure: Modelling tundra PAI with DHP

The main findings of the canopy biophysical analysis (Chapter 4) were as follows.

(1) The results of the canopy structural study showed that DHP can successfully estimate effective PAI (i.e. PAI_e) across a variety of tundra canopy configurations ($r^2=0.86$, $\text{RMSE}=0.15$), in relation to destructively sampled PAI estimates. Further, the DHP CAN-EYE (Wiess et al., 2004) modelling results demonstrated that the use of the Poisson law (Welles & Norman, 1991; Demarez et al., 2008) was more effective than the use of the modified Poisson law (Lang & Yueqin, 1986; Chen & Black, 1992; Demarez et al., 2008) for PAI estimation.

(2) Field-based DHP measurement/modelling demonstrated a latitudinal gradient of PAI_e values, from $\sim 1.14 \text{ m}^2/\text{m}^2$ at lower latitudes to $\sim 0.51 \text{ m}^2/\text{m}^2$ at higher latitudes. Canopy gap fractions also showed a latitudinal gradient, from 0.45 to 0.26 to 0.18 at low, medium and high latitudes, respectively. Latitudinal values of modelled Arctic tundra PAI_e and canopy gap fractions (estimated using the Poisson law) have not been previously reported in the literature. Accordingly, the regional characterization of leaf and canopy structure using DHP in combination with CAN-EYE modelling (Weiss et al., 2004) represented a unique aspect to this research. Knowledge of canopy gap fractions was considered an important component to understanding the spatial variability of the multi-angle spectral sampling and interpreting the results of the empirical and physical modelling.

(3) DHP derived values of (effective) average leaf angle (ALA_e), a leaf and canopy parameter/variable necessary for the PROSAIL RTM modelling, demonstrated a range of values between 10.29° and 79.92° with an average inclination of 52.28° . Such measured/modelled ALA_e values have not been previously available for Arctic canopies. Results such as these are novel for Arctic regions and accordingly offered values for subsequent RTM parametrization.

8.3. Field Scale: Empirical and Physical Modelling

Multi-species, spatially-complex canopies, such as those in the Arctic, test the robustness of optically-based vegetation biochemical and biophysical variable retrieval methods, since the TOC reflectance signal is made up of multiple contributing factors (e.g. various species/pigment pools, non-photosynthetic materials, and soils/mineral substrates/canopy gap fractions). Furthermore, the extreme sun and sensor view zenith angles (VZAs) that are common in the Arctic present an additional confounding factor to variable retrievals since tundra TOC reflectance has been shown to be directionally dependent. Much of Arctic research investigating vegetation variable retrievals

using optical spectroscopic data has not investigated the influence of sensor view angle geometry, nor have any studies fully investigated and compared retrieval methodologies (e.g. parametric regression based on narrowband VIs, non-parametric GPR, or physically based RTMs and inversion strategies) using a high-resolution multi-angle spectroscopic dataset (e.g. Liu et al., 2017; Bartsch et al., 2016). In consideration of the above, the aforementioned empirical and physical modelling methods were investigated for their capability of retrieving LCC, PAI, and CCC from field-scale, multi-angle spectral data acquired across a bioclimatic gradient in the Western Canadian Arctic (see 8.1 (2) above), and thus represented unique aspects of this research. Conclusions drawn from the field-scale modelling were used to inform the modelling approach applied at the remote sensing scale, and further, were considered important for understanding how field-scale measurements (biochemical, biophysical, and spectral) translated/scaled to the remote sensing investigations.

8.3.1. Empirical modelling: Parametric VIs vs. non-parametric GPR

The main findings of the field-scale empirical modelling (Chapter 5) were as follows.

(1) VIs commonly used in the remote sensing literature were assessed for their robustness in predicting LCC, PAI, and CCC across five VZAs (-55° , -36° , 0° , $+36^\circ$, $+55^\circ$) and a variety of environments. The VIs shown to produce the best overall results, inclusive of all VZAs, field sites, and vegetation variables, were SR and ROSAVI, where SR bands were determined through an optimization procedure. The results of the VI assessment showed that systematically running all bands through SR produced better overall results than using a predefined band-set with ROSAVI; however, the multi-band results were not substantially different than those achieved with ROSAVI (e.g. $r^2=0.58$, NRMSE=0.12 vs. $r^2=0.54$, NRMSE=0.16, respectively). These results suggested that

choice of VI formulation may not be as important as the quality of field and spectral data (i.e. sampling gradients should be considered important).

(2) GPR produced the highest correlation-based results compared to the above two VIs, inclusive of all VZAs and vegetation variables ($r^2=0.59$); however, it did not produce the best overall model accuracy (NRMSE=0.16). Moreover, it was shown that the GPR algorithm produced favourable results when used in combination with a spectrally reduced contiguous dataset (i.e. CHRIS/PROBA M1). Like the SR VI, the GPR optimization procedure allowed for the assessment of the physically relevant wavelengths. To date, GPR has not been applied in the Arctic for biophysical and biochemical variable retrievals or for the interpretation of physically meaningful outputs (i.e. spectral bands) as they relate to those variables.

(3) The spectral band selections from both the multi-band SR VI and the GPR modelling outputs were shown to be within physically meaningful wavelength regions. Band selections were typically within the visible (VIS) wavelengths, as they relate to peak green reflectance and pigment absorption, and within the red-edge (RE) and near-infrared (NIR) wavelengths as they relate to leaf and canopy structure. However, meaningful band selections also occurred outside of those ranges; such occurrences may have been attributable to secondary relationships with variables that are said to co-vary with the biochemical and biophysical variables of interest (Ollinger, 2011). Because of the heterogeneous nature of Arctic tundra canopies and the covariation observed across all modelling scenarios, it was difficult if not impossible to define a precise spectral band subset that provided the best predictive power across the study sites. Based on the band selection results of this research, it is therefore recommended that Arctic-based biochemical and biophysical modelling/monitoring efforts not discard spectral bands outside of known absorption/reflectance

ranges. Consequently, the remote sensing analysis was conducted using the fully available band set instead of a few carefully chosen bands.

(4) The SR band assessment showed an observable positive shift in the selection of optimal wavelength regions as VZAs progressed from negative to positive values (i.e. backscatter to forward scatter). This trend was very slight (i.e. almost not detectable) in the GPR optimal band selections. Shifts in VI values (e.g. NDVI values) have been reported for multi-angle spectroscopic studies in other environments (e.g. Galvão et al., 2004) but not for the Arctic.

(5) The results showed that the overall best performing VZA for both parametric and non-parametric retrieval methods was -55° ($r^2=0.52$, NRMSE=0.15); however, results were not significantly different than other VZAs to warrant further investigation into the use of multi-angle field spectroscopy for biochemical and biophysical variable retrievals in Arctic tundra environments. Off-nadir measurements can be used if measurements are kept consistent.

(6) Finally, the results demonstrated that modelling accuracies were best achieved at the plot scale ($>1 \text{ m}^2$) across all model types, vegetation variables, and VZAs. A reduction in subplot variability was determined to be a necessary procedure for improving model outcomes.

8.3.2. Physical modelling and iterative numerical inversion: PROSAIL and LMA

The main findings of the field-scale physical modelling (Chapter 6) were as follows.

(1) The overall modelling results showed that the PROSAIL RTM was capable of simulating the multi-angle TOC spectral-directional reflectance of Arctic tundra ($r^2 \sim 0.99$, RMSE=0.004 $\pm$ 0.002); however, systematic errors (both over and under predictions) were observed across the VIS, RE, and NIR wavelength regions for all sites and VZAs. These errors suggested the following: (a) field spectra contained systematic noise/error that propagated into the curve fitting

procedure, (b) Arctic tundra canopies may (likely) violate the physical assumptions behind the PROSAIL model (i.e. PROSAIL is a turbid medium model, whereas most of the Arctic canopies of this research exhibit complex three-dimensional characteristics, with the exception of Banks Island where the best PROSAIL results were achieved), and (c) model (re)calibration should be explored for Arctic plants/canopies if PROSAIL and its variants are to continue being investigated (e.g. the refractive index and absorption coefficients of leaf constituents should be determined or reconsidered).

(2) The results showed that PROSAIL (inverted with LMA) was not capable of accurately predicting biochemical and biophysical vegetation variables (i.e. LCC, PAI, and CCC) across a diversity of field sites and VZAs in Arctic tundra environments (mean of all modelling results $r^2=0.31$, NRMSE=0.30). Further, the PROSAIL inversions showed that a contiguous narrowband dataset was capable of producing better correlation-based results than a reduced spectral subset containing slightly broader bandwidths ($r^2=0.33$ vs. $r^2=0.28$, respectively), but produced a greater degree of prediction error (NRMSE=0.32 vs. NRMSE=0.29, respectively).

(3) When results were stratified by geographic location, the PROSAIL model produced much better correlation-based results in the high-Arctic sites (a result observed across both field and remote sensing analyses). It is possible that this was an artifact of the field sampling approach in combination with the physical nature of high-Arctic canopies: a more distinctive and detectable gradient existed between the sampled plots than at lower latitudes. This provides an indication that sampling homogenous canopies gives spectra that are too alike to offer differentiation in the estimates (i.e. the ill-posedness factor increases). The geographic variability of the results reinforced the need to test a physical model's applicability/universality across multiple field sites when used in large diverse ecosystems such as the Arctic.

(4) The overall best performing VZA across all field sites and vegetation variables was 0° ($r^2=0.44$, NRMSE=0.28) followed by $+55^\circ$ ($r^2=0.39$, NRMSE=0.30); however, results were not considerably different than the other VZAs when averaged across vegetation variables, field sites, and VZAs. In contrast, PROSAIL demonstrated inconsistent directionally-based results when stratified per vegetation variable and geographic location. It was concluded that the variability of the PROSAIL results was largely related to the inversion approach, and thus ill-posedness remained the biggest factor preventing adequate predictions.

(5) At the commencement of this study LMA had not been used to invert PROSAIL (i.e. in 2011), let alone used to invert multi-angle spectroscopic reflectance data in Arctic environments. Hilker et al. (2017) provided encouraging results with LMA (used in combination with PROSAIL and multi-angle reflectance data) to continue with this approach. However, despite strong spectral curve fitting, overall LMA inversion results were poor. Such results can typically be attributed to model ill-posedness; it is a well-known problem that multiple parameter combinations will lead to the same spectral reflectance (Combal et al., 2002; Darvishzadeh et al., 2008a). LMA was therefore considered extremely susceptible to ill-posedness as only one set of parameters was produced from each inversion. An attempt was made to account for ill-posedness and local minima by employing commonly used regularization strategies, including (a) setting the minimum and maximum values for each parameter based on field measurements and accepted ranges based on the literature, (b) setting algorithm start values based on average leaf/canopy conditions, and (c) fixing algorithm variables with known fixed parameters (e.g. VZAs). Inverted values obtained at the field-scale were used to further constrain the inversion at the remote sensing level.

8.4. Remote Sensing Scale: Empirical and Physical Modelling

To the author's knowledge, empirical and physical modelling methods have not been investigated or compared for their retrieval capabilities with spaceborne multi-angle imaging spectroscopy data acquired in Arctic tundra environments (e.g. Liu et al., 2017; Bartsch et al., 2016). To address this research gap, the empirical (i.e. parametric regression based on SR and ROSAVI and non-parametric GPR) and physical methods (i.e. inversion of PROSAIL using LMA) investigated at the field-scale were compared for their capability of retrieving LCC, PAI, and CCC from multi-angle CHRIS/PROBA Mode-1 imagery acquired across a bioclimatic gradient in the Western Canadian Arctic (see 8.1 (3) above). The main findings of the remote sensing empirical and physical modelling study (Chapter 7) were as follows.

(1) The results showed that iteration-based empirical modelling methodologies (i.e. SR and GPR) produced the best overall outcomes across all vegetation variables, field sites, and VZAs. The highest correlation based results were achieved with GPR ($r^2=0.59$) followed by SR ($r^2=0.53$); however, best predictive performance was achieved by SR (NRMSE=0.14) followed by GPR (NRMSE=0.16).

(2) The results showed that, like the field-based approach, the CHRIS/PROBA spectral band selections from both SR and GPR modelling outputs were within physically meaningful wavelength regions that related to the variables of interest (i.e. LCC, PAI, and CCC). Important spectral band selections were similar to those selected at the field-scale and some meaningful band selections also occurred outside of those ranges (i.e. due to variable covariation), thus providing further evidence of the benefit of using contiguous spectroscopic bands for biochemical and biophysical variable retrievals in Arctic environments. Like the empirical field-based analysis, a very slight trend (almost undetectable) in spectral band selections was observed with changing

VZAs; however, unlike the field-based analysis, the observed shift in band selections were opposite to that observed at the field scale.

(3) Use of preselected wavelengths in a soil-based VI (i.e. ROSAVI) produced the overall least accurate fits/model predictions ($r^2=0.48$, NRMSE=0.17); however, results were not substantially different from those obtained with SR and GPR. As ROSAVI was the simplest and quickest to implement, its utility for rapid variable retrievals was demonstrated. Further investigation into the use of soil-based narrowband VIs is warranted due to the prevalence of gap fractions and non-photosynthetic materials found in Arctic tundra canopies.

(4) PROSAIL was capable of simulating CHRIS/PROBA TOC spectral-directional reflectance ($r^2 \sim 0.99$, RMSE=0.005 $\pm$ 0.005); however, a similar but more distinctive systematic error pattern was observed across the VIS, RE, and NIR wavelength regions for all sites and VZAs. These distinct patterns emerged in the following regions: wavelengths less than ~ 500 nm (over prediction), peak green reflectance centered at ~ 551 nm (over prediction), pigment absorption centered at ~ 680 nm (under prediction), wavelengths in the RE and NIR between ~ 700 nm to 750 nm (over prediction), reflectance in the NIR centered at ~ 785 nm (under prediction), and wavelengths greater than 990 nm (over prediction).

(5) The results of the LMA inversion demonstrated that LCC, PAI, and CCC cannot be estimated with accuracies comparable to those achieved with the empirical approaches. Inversion of PROSAIL yielded an overall correlation of $r^2=0.28$ and an overall accuracy of NRMSE=0.27 irrespective of vegetation variable, VZA, and geographic location. Furthermore, regularization strategies applied to the LMA inversion (e.g. use of the mean values and constrained ranges of the inverted parameters found in the field scale analysis) did not ameliorate correlation based results ($r^2=0.25$), but slightly improved prediction accuracies (NRMSE=0.25).

(6) The overall best performing VZA for both empirical and physical modelling approaches was $+55^\circ$ ($r^2=0.45$, $\text{NRMSE}=0.19$), while nadir (0°) VZAs produced the worst model outcomes (mean $r^2=0.33$, $\text{NRMSE}=0.18$). Overall, the combined prediction accuracies for all VZAs were very similar ($\text{NRMSE}=0.18\pm0.01$), indicating no distinct advantage for any one VZA. In comparison, the field-based multi-angle prediction results also showed almost identical accuracies ($\text{NRMSE}=0.19\pm0.01$),

(7) Finally, the remote sensing empirical and physical modelling results produced very similar outcomes to the field-based modelling results obtained in Chapters 5 and 6, thus providing confirmation that the spatial sampling and spectral resampling methodology employed at the field scale was appropriate for scaling to the remote sensing level.

8.5. Statistical Assessment of Model and View Angle Performance

The results of the field and remote sensing scale empirical and physical modelling analyses were combined and statistically assessed using a one-way analysis of variance (ANOVA) to determine if there were any significant differences between modelling methods (i.e. is there a modelling method that provides a statistically significant advantage over the others?) and to determine if there was a statistically significant advantage to using a multi-angle approach for estimating vegetation variables in the Arctic (i.e. is there a VZA that provides a statistically significant advantage over other VZAs?). ANOVA modelling was carried out using an alpha level of 0.05. Each ANOVA test was followed by a Tukey post-hoc test to determine where significant differences occur between test groups. Results for each vegetation variable were combined into one value for both the model and angle assessments. ANOVA testing was completed in SPSS Statistics 24.0 (IBM Corporation, 2016).

8.5.1. Model performance

Tables 43-45 give, respectively, the descriptive statistics (based on r^2) for each modelling method, results of the ANOVA, and the Tukey post-hoc results. The ANOVA showed that there were significant differences between the modelling methods ($p < 0.05$, $F = 90.44$), while the post-hoc Tukey test showed that GPR produced significantly better results than ROSAVI and PROSAIL, but was not significantly better than the SR VI.

Table 43 Descriptive statistics for combined model-based results (r^2) for plot scale assessments (all angles combined, all locations combined, and both sensors combined).

<i>Test</i>	<i>Count (n)</i>	<i>Mean r^2</i>	<i>Std. Dev.</i>	<i>Std. Err.</i>	<i>95% Confidence Interval</i>			
					<i>Lower</i>	<i>Upper</i>	<i>Min</i>	<i>Max</i>
<i>SR</i>	183	0.55	0.19	0.01	0.52	0.57	0.12	0.96
<i>ROSAVI</i>	183	0.52	0.18	0.01	0.49	0.54	0.16	0.94
<i>GPR</i>	183	0.59	0.17	0.01	0.57	0.62	0.21	0.96
<i>PROSAIL</i>	186	0.30	0.21	0.02	0.27	0.33	0.00	0.80
<i>Total</i>	735	0.49	0.22	0.01	0.47	0.50	0.00	0.96

Table 44 ANOVA results for model comparisons based on r^2 . Results are significant at the 0.05 level.

<i>Test</i>	<i>Sum of squares</i>	<i>Degrees of freedom</i>	<i>Mean square</i>	<i>F</i>	<i>Significance</i>
<i>Between groups</i>	9.53	3.00	3.18	90.44	0.00
<i>Within groups</i>	25.68	731.00	0.04		
<i>Total</i>	35.22	734.00			

Table 45 Tukey's post-hoc test for model comparisons based on r^2 . Significant *I-J* mean differences are bolded. The mean difference is significant at the 0.05 level.

<i>Test (I)</i>	<i>Test (J)</i>	<i>Mean Difference (I-J)</i>	<i>Std. Err.</i>	<i>Significance</i>	<i>95% Confidence Interval</i>	
					<i>Lower</i>	<i>Upper</i>
<i>SR</i>	<i>ROSAVI</i>	0.03	0.02	0.51	-0.02	0.08
	<i>GPR</i>	-0.05	0.02	0.10	-0.10	0.01
	<i>PROSAIL</i>	0.25	0.02	0.00	0.20	0.30
<i>ROSAVI</i>	<i>SR</i>	-0.03	0.02	0.51	-0.08	0.02
	<i>GPR</i>	-0.07	0.02	0.00	-0.12	-0.02
	<i>PROSAIL</i>	0.22	0.02	0.00	0.17	0.27
<i>GPR</i>	<i>SR</i>	0.05	0.02	0.10	-0.01	0.10
	<i>ROSAVI</i>	0.07	0.02	0.00	0.02	0.12
	<i>PROSAIL</i>	0.29	0.02	0.00	0.24	0.34
<i>PROSAIL</i>	<i>SR</i>	-0.25	0.02	0.00	-0.30	-0.20
	<i>ROSAVI</i>	-0.22	0.02	0.00	-0.27	-0.17
	<i>GPR</i>	-0.29	0.02	0.00	-0.34	-0.24

Tables 46-48 give, respectively, the descriptive statistics (based on prediction accuracy, NRMSE) for each modelling method, results of the ANOVA, and the Tukey post-hoc results. The ANOVA showed significant differences in prediction performance between methods, with the post-hoc test showing that SR produced significantly better predictions than GPR, ROSAVI, and PROSAIL. Surprisingly, GPR and ROSAVI produced accuracies that showed no statistical difference.

Table 46 Descriptive statistics for combined model-based results (NRMSE) for plot scale assessments (all angles combined, all locations combined, and both sensors combined).

<i>Test</i>	<i>Count (n)</i>	<i>Mean NRMSE</i>	<i>Std. Dev.</i>	<i>Std. Err.</i>	<i>95% Confidence Interval</i>			
					<i>Lower</i>	<i>Upper</i>	<i>Min</i>	<i>Max</i>
<i>SR</i>	183	0.13	0.05	0.00	0.12	0.14	0.05	0.26
<i>ROSAVI</i>	183	0.16	0.06	0.00	0.15	0.17	0.06	0.36
<i>GPR</i>	183	0.16	0.06	0.00	0.15	0.17	0.06	0.30
<i>PROSAIL</i>	186	0.29	0.13	0.01	0.27	0.31	0.09	0.67
<i>Total</i>	735	0.19	0.10	0.00	0.18	0.19	0.05	0.67

Table 47 ANOVA results for model comparisons based on NRMSE. Results are significant at the 0.05 level.

<i>Test</i>	<i>Sum of squares</i>	<i>Degrees of freedom</i>	<i>Mean square</i>	<i>F</i>	<i>Significance</i>
<i>Between groups</i>	2.90	3.00	0.97	136.85	0.00
<i>Within groups</i>	5.16	731.00	0.01		
<i>Total</i>	8.05	734.00			

Table 48 Tukey's post-hoc test for model comparisons based on NRMSE. Significant *I-J* mean differences are bolded. The mean difference is significant at the 0.05 level.

<i>Test (I)</i>	<i>Test (J)</i>	<i>Mean Difference (I-J)</i>	<i>Std. Err.</i>	<i>Significance</i>	<i>95% Confidence Interval</i>	
					<i>Lower</i>	<i>Upper</i>
<i>SR</i>	<i>ROSAVI</i>	-0.03	0.01	0.00	-0.05	-0.01
	<i>GPR</i>	-0.03	0.01	0.00	-0.05	-0.01
	<i>PROSAIL</i>	-0.16	0.01	0.00	-0.18	-0.14
<i>ROSAVI</i>	<i>SR</i>	0.03	0.01	0.00	0.01	0.05
	<i>GPR</i>	0.00	0.01	1.00	-0.02	0.02
	<i>PROSAIL</i>	-0.13	0.01	0.00	-0.15	-0.11
<i>GPR</i>	<i>SR</i>	0.03	0.01	0.00	0.01	0.05
	<i>ROSAVI</i>	0.00	0.01	1.00	-0.02	0.02
	<i>PROSAIL</i>	-0.13	0.01	0.00	-0.15	-0.11
<i>PROSAIL</i>	<i>SR</i>	0.16	0.01	0.00	0.14	0.18
	<i>ROSAVI</i>	0.13	0.01	0.00	0.11	0.15
	<i>GPR</i>	0.13	0.01	0.00	0.11	0.15

8.5.2. Multi-angle performance

Tables 49-51 give the descriptive statistics (based on r^2 for the different VZAs), the ANOVA, and the Tukey post-hoc results, respectively, over all modelling methods, sites and sensors. The results of the ANOVA (using combined r^2 modelling values) showed that there were no significant differences between VZAs ($p>0.05$, $F=0.89$).

Table 49 Descriptive statistics for VZA-based test results (r^2) for plot scale assessments (all tests combined, all locations combined, and both sensors combined).

VZA	Count (n)	Mean r^2	Std. Dev.	Std. Err.	95% Confidence Interval		Min	Max
					Lower	Upper		
0°	168	0.51	0.20	0.02	0.48	0.54	0.00	0.87
-36°	144	0.47	0.24	0.02	0.43	0.51	0.01	0.93
-55°	135	0.49	0.23	0.02	0.45	0.53	0.01	0.96
+36°	144	0.47	0.22	0.02	0.43	0.50	0.01	0.96
+55°	144	0.50	0.22	0.02	0.46	0.53	0.00	0.88
Total	735	0.49	0.22	0.01	0.47	0.50	0.00	0.96

Table 50 ANOVA results for VZA comparisons based on r^2 . Results are significant at the 0.05 level.

VZA	Sum of squares	Degrees of freedom	Mean square	F	Significance
Between groups	0.17	4	0.04	0.89	0.47
Within groups	35.04	730	0.05		
Total	35.22	734			

Table 51 Tukey's post-hoc test for VZA comparisons based on r^2 . Significant *I-J* mean differences are bolded. The mean difference is significant at the 0.05 level.

VZA (I)	VZA (J)	Mean Difference (I-J)	Std. Err.	Significance	95% Confidence Interval	
					Lower	Upper
0°	-36°	0.03	0.02	0.64	-0.03	0.10
	-55°	0.02	0.03	0.94	-0.05	0.09
	+36°	0.04	0.02	0.45	-0.03	0.11
	+55°	0.01	0.02	0.99	-0.06	0.08
-36°	0°	-0.03	0.02	0.64	-0.10	0.03
	-55°	-0.01	0.03	0.98	-0.09	0.06
	+36°	0.01	0.03	1.00	-0.06	0.08
	+55°	-0.02	0.03	0.91	-0.09	0.05
-55°	0°	-0.02	0.03	0.94	-0.09	0.05
	-36°	0.01	0.03	0.98	-0.06	0.09
	+36°	0.02	0.03	0.92	-0.05	0.09
	+55°	-0.01	0.03	1.00	-0.08	0.06
+36°	0°	-0.04	0.02	0.45	-0.11	0.03

	-36°	-0.01	0.03	1.00	-0.08	0.06
	-55°	-0.02	0.03	0.92	-0.09	0.05
	+55°	-0.03	0.03	0.79	-0.10	0.04
+55°	0°	-0.01	0.02	0.99	-0.08	0.06
	-36°	0.02	0.03	0.91	-0.05	0.09
	-55°	0.01	0.03	1.00	-0.06	0.08
	+36°	0.03	0.03	0.79	-0.04	0.10

The best performing VZA for all field sites, vegetation variables, and modelling methods was 0° (NRMSE=0.18); all other VZAs produced slightly lower but equal accuracies (NRMSE=0.19). Descriptive statistics (based on the NRMSE), results of ANOVA, and the Tukey post-hoc results can be found in Tables 52-54, respectively. ANOVA showed that there were no significant differences between VZAs ($p>0.05$, $F=0.48$).

Table 52 Descriptive statistics for VZA-based test results (NRMSE) for plot scale assessments (all tests combined, all locations combined, and both sensors combined).

<i>VZA</i>	<i>Count (n)</i>	<i>Mean NRMSE</i>	<i>Std. Dev.</i>	<i>Std. Err.</i>	<i>95% Confidence Interval</i>			
					<i>Lower</i>	<i>Upper</i>	<i>Min</i>	<i>Max</i>
0°	168	0.18	0.11	0.01	0.16	0.20	0.06	0.65
-36°	144	0.19	0.11	0.01	0.18	0.21	0.05	0.62
-55°	135	0.19	0.10	0.01	0.17	0.20	0.06	0.62
+36°	144	0.19	0.11	0.01	0.17	0.21	0.05	0.67
+55°	144	0.19	0.10	0.01	0.17	0.20	0.06	0.66
Total	735	0.19	0.10	0.00	0.18	0.19	0.05	0.67

Table 53 ANOVA results for VZA comparisons based on NRMSE. Results are significant at the 0.05 level.

<i>VZA</i>	<i>Sum of squares</i>	<i>Degrees of freedom</i>	<i>Mean square</i>	<i>F</i>	<i>Significance</i>
<i>Between groups</i>	0.02	4.00	0.01	0.48	0.75
<i>Within groups</i>	8.03	730.00	0.01		
<i>Total</i>	8.05	734.00			

Table 54 Tukey's post-hoc test for VZA comparisons based on NRMSE. Significant *I-J* mean differences are bolded. The mean difference is significant at the 0.05 level.

<i>VZA (I)</i>	<i>VZA (J)</i>	<i>Mean Difference (I-J)</i>	<i>Std. Err.</i>	<i>Significance</i>	<i>95% Confidence Interval</i>	
					<i>Lower</i>	<i>Upper</i>
0°	-36°	-0.01	0.01	0.75	-0.05	0.02
	-55°	-0.01	0.01	0.98	-0.04	0.03
	+36°	-0.01	0.01	0.78	-0.05	0.02
	+55°	-0.01	0.01	0.97	-0.04	0.02
-36°	0°	0.01	0.01	0.75	-0.02	0.05

	-55°	0.01	0.01	0.98	-0.03	0.04
	+36°	0.00	0.01	1.00	-0.03	0.03
	+55°	0.01	0.01	0.99	-0.03	0.04
-55°	0°	0.01	0.01	0.98	-0.03	0.04
	-36°	-0.01	0.01	0.98	-0.04	0.03
	+36°	-0.01	0.01	0.99	-0.04	0.03
	+55°	0.00	0.01	1.00	-0.03	0.03
+36°	0°	0.01	0.01	0.78	-0.02	0.05
	-36°	0.00	0.01	1.00	-0.03	0.03
	-55°	0.01	0.01	0.99	-0.03	0.04
	+55°	0.01	0.01	0.99	-0.03	0.04
+55°	0°	0.01	0.01	0.97	-0.02	0.04
	-36°	-0.01	0.01	0.99	-0.04	0.03
	-55°	0.00	0.01	1.00	-0.03	0.03
	+36°	-0.01	0.01	0.99	-0.04	0.03

8.6. Overall Conclusions and Contributions

The primary research question asked in this thesis was: Can spectroscopic multi-angular imagery from the CHRIS/PROBA sensor be used to retrieve biochemical and biophysical variables, specifically leaf chlorophyll content (LCC), plant area index (PAI), and canopy chlorophyll content (CCC) at the remote sensing scale in the Western Canadian Arctic and does a multi-angular spectroscopic remote sensing approach provide any benefit for vegetation variable retrieval over nadir looking spectroscopic instruments? It has been concluded through both the field and remote sensing based studies that multi-angle remote sensing does not provide a statistically significant benefit over nadir looking instruments for the retrieval of leaf and canopy biochemical and biophysical variables in tundra environments where extreme sun-target-sensor geometries are common, and thus this study alleviates some doubt surrounding this question. This result can be interpreted as, any/all remote sensing acquisitions (i.e. any unique angle within the angular confines of those investigated here; e.g. VZAs within $\pm 55^\circ$) provide comparable characterizations of vegetated surfaces when using small footprint spectroscopic sensors (such as the one used in this study) and are therefore equally suitable for biochemical and biophysical variable retrievals in the Arctic. This question was investigated through evaluation of two groups

of modelling methodologies: empirical and physical. Hence, the second major undertaking and secondary major research questions of this thesis pertained to providing a comparison of vegetation variable retrieval methods using multi-angle multi-scale spectroscopic data measured across a bioclimatic gradient.

It has been concluded that iteration based empirical methods were the most effective methods for retrieving biochemical and biophysical vegetation variables from multi-angle spectroscopic optical data in Arctic tundra ecosystems irrespective of view angle and spatial scale. Machine learning regression (i.e. GPR) produced the best correlation-based results, however, the multi-band vegetation index (i.e. SR) was shown to provide statistically comparable results while providing a more simplistic/transparent methodological approach. Moreover, the SR approach produced statistically significant superior prediction accuracies. A benefit of using both empirically based GPR and VI methods is that they provide physically meaningful outputs (i.e. prediction bands/wavelengths that can be linked to the variable of interest). Selection of the SR VI method over the GPR approach may come down to model simplicity and ease of implementation. Although results were comparable between these methods, the slight statistical advantage of the SR VI may provide more impactful variable estimations when applied over broad spatial and temporal scales. Furthermore, modelled band selections showed that narrow absorption/reflectance features and variable covariation is an important consideration when constructing reflectance models used for biophysical and biochemical vegetation variable retrievals in the Arctic, and thus it can be concluded that full spectrum (e.g. 400 nm to 1000 nm), contiguous narrowband imaging spectroscopy may provide benefits over multispectral imaging for such tasks.

The results of the physical modelling demonstrated that Arctic tundra leaf and canopy biochemical and biophysical variables cannot be accurately predicted through the inversion of the

PROSAIL one-dimensional RTM using the Levenberg-Marquardt iterative numerical optimization algorithm. Although acceptable modelling results (albeit with large positive biases) were achieved in a high Arctic location, the combined latitudinal results highlight the importance of sampling and testing across multiple field sites, especially with generally-applicable physical modelling approaches. The LMA inversion of PROSAIL was shown to accurately simulate TOC spectral reflectance; however, poor predictions clearly demonstrate the problem of ill-posedness and model calibration.

The results, when analyzed geographically, demonstrate how canopy complexity (i.e. both horizontal and vertical complexity) and vegetation cover gradients (i.e. spatial variability in percent vegetation cover) can play a large role in vegetation variable retrievals in the Arctic. For example, the best modelling results (regardless of model) were achieved in the high Arctic (Banks Island) where canopy complexity was lower overall (i.e. canopies were two-dimensional in nature), spatial differences between sparsely vegetated and fully vegetated canopies were more pronounced, and average canopy gap fractions were generally greater. In comparison, the vegetation canopies of the lower latitude sites (Herschel Island, Richards Island, and Richardson Mountains) possessed an overall greater canopy complexity (i.e. canopies were more three-dimensional in nature), exhibited fewer canopy gaps, and were more spatially continuous/contiguous (i.e. average percent cover was greater overall). Recommendations for those conducting biochemical and biophysical variable retrievals in the Arctic are as follows. First, an emphasis should be placed on capturing vegetation gradients whether working in low or high Arctic ecosystems (a feat more easily accomplished in the high Arctic). Field sampling should be conducted across the full range of vegetation conditions and canopy configurations and should not focus solely on sampling similar monotypic or continuous/contiguous vegetation assemblages (i.e.

where there is low landscape-scale spatial variability). The importance of sampling gradients is exemplified in the results of this study. Capturing these gradients in low-Arctic sites may help overcome the limitations imposed by more complex three-dimensional canopies. Secondly (and tied to the previous point), in any remote sensing-based vegetation variable retrieval study, a strong emphasis should be placed on capturing high-quality, representative field data. As simple as it might seem, data plays an important (if not the most important) role in any modelling scenario – almost more so than the chosen modelling approach. Similar results between the SR and GPR modelling methods in this study point towards the limitations that field data, as collected for each of the field sites, can impose upon modelling outcomes. The adage “garbage in, garbage out” should not be forgotten. Given that this project served primarily as an adaptation of established empirical and physical methods to Arctic environments using multi-angle spectroscopic reflectance data, there is ample opportunity to explore additional full spectrum modelling approaches (e.g. machine learning regression algorithms will likely become more accurate as more training data are made available) and new hyperspectral sensors as they become available (e.g. the Environmental Mapping and Analysis Program, or EnMap; Kaufmann et al., 2006). Although the physical modelling approach produced the least favorable results, it should not be abandoned as, in theory, it could eventually provide a universal retrieval approach.

In addition to the leaf and canopy physical model selected for this research (i.e. PROSAIL), there are opportunities to explore other RTMs (e.g. Widlowski et al., 2013). Certainly, three-dimensional RTMs that are better suited for describing abstract heterogeneous canopies with anisotropic backgrounds may be of more use in tundra environments. Furthermore, there is ample opportunity to explore the use of alternative inversion procedures, such as look-up-tables and artificial neural networks, as these may outcompete iterative numerical optimization. Finally, the

full spectrum data that include short-wavelength infrared regions may provide additional benefits for retrieving and mapping biochemical and biophysical variables in Arctic environments and should be explored.

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Appendix A: Multi-band Vegetation Indices

Available at: <https://doi.org/10.6084/m9.figshare.5794638.v1>

Appendix B: Narrowband Vegetation Indices

Available at: <https://doi.org/10.6084/m9.figshare.5794701.v1>

Appendix C: Machine Learning Regression Algorithms

Available at: <https://doi.org/10.6084/m9.figshare.5794722.v1>

Appendix D: PROSAIL Simple Sensitivity Analysis

A simple sensitivity analysis was performed with the PROSAIL radiative transfer model (RTM) (Jacquemoud et al., 2009) using all 14 leaf and canopy parameters. Sensitivity analyses are useful for providing insight into the functioning of RTMs by identifying the key input variables (i.e. biochemical and biophysical properties) that drive spectral outputs (i.e. top of canopy [TOC] reflectance). Further, sensitivity analyses can help give insight into which variables explain most of the variability in the reflectance field. This analysis was completed to qualitatively evaluate (a) the influence that view zenith angle (VZA) (i.e. directional reflectance) plays on the output of each of the iterated leaf and canopy parameters, and (b) the influence (i.e. contributions) that each of the leaf and canopy parameters have on the directional reflectance variability.

The sensitivity analysis was performed by varying two parameters combinations while holding the remaining parameters constant, although such an assumption is unlikely under natural conditions as biochemical and biophysical parameters often co-vary (Jacquemoud et al., 2009). Parameter start values and parameter ranges were based on field data and accepted values found in the literature (see Table 33, Chapter 6). In addition to those values listed, a constant sun zenith angle (SZA) of 56° and relative azimuth angle (RAA) of 0° was used (except when iterated). For each of the parameters, iterations were performed spanning the expected ranges of the data (i.e. min to max) over five view zenith angles (VZAs): -55° , -36° , 0° , $+36^\circ$, $+55^\circ$.

The outputs of the sensitivity analysis are shown in the Figures 90 to 102 below. Overall, it was demonstrated that VZA plays a large role in TOC reflectance across all wavelength regions (i.e. 400 nm to 1000 nm) with greater reflectance values generally appearing in backscatter VZAs. Short descriptions of each leaf and canopy's parameter influences on TOC follow.

Figure 90 PROSAIL iterations based on the leaf structure parameter (N) and VZA. From top left: (1) TOC reflectance for each parameter combination, (2) coefficient of variation of combined N values per VZA (i.e. all N values averaged and then stratified by VZA), and (3) coefficient of variation of combined VZAs values per N value range/classes.

Leaf structure (N) based reflectance variability was shown to be highly influenced by VZA (Figure 90), with greatest variability observed in the peak green reflectance (~ 550 nm) and in the near-infrared (NIR, $> \sim 700$ nm) regions. The observed variability can be attributed to: (a) backscatter reflectance, and (b) high N values or the complete absence thereof (i.e. greater degree of structure vs. the influence of soil/background reflectance).

Figure 91 PROSAIL iterations based on the leaf chlorophyll content (C_{ab}) and VZA. From top left: (1) TOC reflectance for each parameter combination, (2) coefficient of variation of combined C_{ab} values per VZA (i.e. all C_{ab} values averaged and then stratified by VZA), and (3) coefficient of variation of combined VZAs values per C_{ab} value range/classes.

Leaf chlorophyll content (C_{ab}) based reflectance variability was shown to be highly influenced by VZA (Figure 91), with the greatest variability observed in the chlorophyll absorption regions (~680 nm). The observed variability can be attributed to: (a) backscatter reflectance and (b) high C_{ab} values (i.e. greater degree of pigments) or the complete absence thereof (the influence of background/soil reflectance begins to manifest in the TOC signal).

Figure 92 PROSAIL iterations based on the leaf carotenoid content (C_{ar}) and VZA. From top left: (1) TOC reflectance for each parameter combination, (2) coefficient of variation of combined C_{ar} values per VZA (i.e. all C_{ar} values averaged and then stratified by VZA), and (3) coefficient of variation of combined VZAs values per C_{ar} value range/classes.

Leaf carotenoid content (C_{ar}) based reflectance variability was shown to be moderately influenced by VZA (Figure 92), with the greatest variability observed in the carotenoid absorption regions (~ 520 nm). The observed variability can be attributed to: (a) backscatter reflectance and (b) high C_{ar} values (i.e. greater degree of pigments) or the complete absence thereof. Overall, C_{ar} appears to have very small influence on modelled TOC reflectance.

Figure 93 PROSAIL iterations based on the leaf brown pigment content (C_{bp}) and VZA. From top left: (1) TOC reflectance for each parameter combination, (2) coefficient of variation of combined C_{bp} values per VZA (i.e. all C_{bp} values averaged and then stratified by VZA), and (3) coefficient of variation of combined VZAs values per C_{bp} value range/classes.

Leaf brown pigment (C_{bp}) based reflectance variability was shown to be moderately influenced by VZA (Figure 93), with greatest variability observed in the peak green reflectance (~ 550 nm) and in the near-infrared (NIR, ~ 750 nm). The observed variability can be attributed to: (a) backscatter reflectance (b) high C_{bp} values in the visible (VIS) wavelengths, and (c) low C_{bp} values in the NIR wavelengths.

Figure 94 PROSAIL iterations based on the leaf equivalent water thickness content (C_w) and VZA. From top left: (1) TOC reflectance for each parameter combination, (2) coefficient of variation of combined C_w values per VZA (i.e. all C_w values averaged and then stratified by VZA), and (3) coefficient of variation of combined VZAs values per C_w value range/classes.

Leaf equivalent water thickness (C_w) based reflectance variability was shown to be somewhat influenced by VZA (Figure 94), with the greatest variability observed in the $>\sim 940$ nm wavelength region. The observed variability can be attributed to: (a) backscatter reflectance (i.e. the greatest reflectance values), and (b) low C_w values (i.e. less spectral absorption). C_w was shown to exert overall little influence on modelled TOC reflectance variability.

Figure 95 PROSAIL iterations based on the leaf mass/dry matter content (C_m) and VZA. From top left: (1) TOC reflectance for each parameter combination, (2) coefficient of variation of combined C_m values per VZA (i.e. all C_m values averaged and then stratified by VZA), and (3) coefficient of variation of combined VZAs values per C_m value range/classes.

Leaf mass (C_m) based reflectance variability was shown to be moderately influenced by VZA (Figure 95), with the greatest variability observed in the peak green reflectance (~ 550 nm) and in the near-infrared (NIR, $> \sim 700$ nm). The observed variability can be attributed to: (a) backscatter reflectance, and (b) low C_m values (i.e. low leaf mass absorption values would decrease pigment related absorption and increase background reflectance values in the NIR).

Figure 96 PROSAIL iterations based on the leaf area index (LAI) and VZA. From top left: (1) TOC reflectance for each parameter combination, (2) coefficient of variation of combined LAI values per VZA (i.e. all LAI values averaged and then stratified by VZA), and (3) coefficient of variation of combined VZAs values per LAI value range/classes.

Leaf area index (LAI) based reflectance variability was shown to be very highly influenced by VZA (Figure 96), with the greatest variability observed in most wavelength regions below $\sim 700\text{nm}$ and lower variability in the NIR regions. The observed variability can be attributed to: (a) backscatter reflectance, though variability was especially high at 0° , and (b) high(er) LAI values. Such a result highlights the combined importance of canopy gap fractions and VZAs.

Figure 97 PROSAIL iterations based on the average leaf angle (ALA) and VZA. From top left: (1) TOC reflectance for each parameter combination, (2) coefficient of variation of combined ALA values per VZA (i.e. all ALA values averaged and then stratified by VZA), and (3) coefficient of variation of combined VZAs values per ALA value range/classes.

Like LAI, average leaf angle (ALA) based reflectance variability was also shown to be highly influenced by VZA (Figure 97), with the greatest variability observed in wavelength regions below ~700 nm and lower variability in the NIR. The observed variability can be attributed: (a) forward scatter reflectance (with very low backscatter variability), and (b) high ALA values ($\geq 60^\circ$). This result demonstrates the theoretical importance of ALA to directional TOC reflectance.

Figure 98 PROSAIL iterations based on the hot spot parameter (S_L) and VZA. From top left: (1) TOC reflectance for each parameter combination, (2) coefficient of variation of combined S_L values per VZA (i.e. all S_L values averaged and then stratified by VZA), and (3) coefficient of variation of combined VZAs values per S_L value range/classes.

Hot spot (S_L) based reflectance variability was shown to be moderately influenced by VZA (Figure 98), with slightly greater variability observed in the VIS wavelength regions below ~700 nm. The observed variability can be attributed to: (a) backscatter reflectance (with zero influence at forward scatter reflectance), and (b) low S_L values (especially in the VIS). The overall influence of S_L to TOC reflectance was mostly low and uniform across all spectral regions.

Figure 99 PROSAIL iterations based on soil reflectance (P_s) and VZA. From top left: (1) TOC reflectance for each parameter combination, (2) coefficient of variation of combined P_s values per VZA (i.e. all P_s values averaged and then stratified by VZA), and (3) coefficient of variation of combined VZAs values per P_s value range/classes.

Soil reflectance (P_s) based reflectance variability was shown to be highly influenced by VZA (Figure 99), with the greatest variability observed in wavelength below ~ 700 nm. The overall observed variability can be attributed to: (a) forward scatter reflectance (especially in the VIS), and (b) low P_s values (in the NIR). The importance of soil-based contributions to overall TOC reflectance variability is apparent for both positive VZAs and low P_s values.

Figure 100 PROSAIL iterations based on the ratio of diffuse radiation (SKYL) and VZA. From top left: (1) TOC reflectance for each parameter combination, (2) coefficient of variation of combined SKYL values per VZA (i.e. all SKYL values averaged and then stratified by VZA), and (3) coefficient of variation of combined VZAs values per SKYL value range/classes.

The diffuse radiation (SKYL) based reflectance variability was shown to be moderately influenced by VZA (Figure 100). The overall observed variability can be attributed to: (a) extreme forward and backscatter reflectance ($\pm 55^\circ$), (b) low SKYL values (all wavelengths), and (c) high SKLY values (i.e. high variability at <520 nm, 680 nm, and <710 nm).

Figure 101 PROSAIL iterations based on solar zenith angle (SZA) and VZA. From top left: (1) TOC reflectance for each parameter combination, (2) coefficient of variation of combined SZA values per VZA (i.e. all SZA values averaged and then stratified by VZA), and (3) coefficient of variation of combined VZAs values per SZA value range/classes.

Solar zenith angle (SZA) based reflectance variability was shown to be moderately influenced by VZA (Figure 101), with a slightly greater degree of variability observed in the VIS wavelength regions below ~ 700 nm. The observed variability can be attributed to: (a) extreme backscatter reflectance (-55°), (b) low SZA values in the VIS, (c) median SZA values (55° , oddly enough), and (d) high SZA values in the NIR.

Figure 102 PROSAIL iterations based on relative azimuth angle (RAA) and VZA. From top left: (1) TOC reflectance for each parameter combination, (2) coefficient of variation of combined RAA values per VZA (i.e. all RAA values averaged and then stratified by VZA), and (3) coefficient of variation of combined VZAs values per RAA value range/classes.

Relative azimuth angle (RAA) based reflectance variability was shown to be moderately influenced by VZA (Figure 102). The observed variability can be attributed to: (a) extreme backscatter reflectance (-55°), (b) low RAA values (in the NIR), and (c) RAA values $\geq 45^\circ$ (particularly in 680 nm and <500 nm).