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Hyperspectral Algorithms

Report in the frame of EnMAP
preparation activities

Scientific Technical Report STR10/08

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Introduction

Against the background of EnMAP preparation analyses have been carried out on the status of research in various areas of hyperspectral remote sensing for the use of existing algorithms in the EnMAP application box. The aim was to compose the status of research in Germany and internationally. Therefore, in various fields of expertise applied and accordingly available algorithms and products based on hyperspectral data has been evaluated and documented. The intention has been to demonstrate and to evaluate the added value of hyperspectral remote sensing to multispectral methods for each product. For this purpose analyses have been carried out by different research groups which were based on the specialty and the experience of each group. Hereby a summary was created of each major application perspective and the relevant remote sensing derived variables and significant processing algorithms (state-of-the-art) belonging to this context. Based on this, the research delivers, as a result, a recommendation which of the algorithms should be implemented into the Applikationsbox of EnMAP. Tests of the algorithms or their implementation were not part of the analyses. However, notes have been given on what algorithms should be tested in the context of a detailed preparation phase. An assessment to the further R & D requirements in the development of algorithms has been made on this basis.

The selection and evaluation of the references **followed the following** premises:

- The algorithms selected should use particular properties of a hyperspectral sensor
- The techniques for information gathering should be as precise as possible.
- The algorithms should be transferable (spatial and temporal).
- The methods should be automatable.
- The methods should be common.
- The algorithms need to be relevant as possible for the use in their field of expertise and need to provide information that is required by the user.
- If additional data is needed to use the algorithm, these should be listed and their availability should be taken in account.
- Similar approaches need to be evaluated in terms of their advantages and disadvantages.
- The methodology is available for a possible implementation in the application box of EnMAP. (License requirements, source code availability, availability as a DLL or executable file).

The literature has generally taken into account the past ten years and if needed, it includes previous periods, too. To support the preparations for the first national workshop publications of German scientists / institutions have been acknowledged separately. The annex to this draft provides the categorized list of publications.

The analyses have been carried out in six subject areas:

- Geology / soils
- Agricultural land use
- Generic algorithms.
- Waters
- Artificial surfaces
- Forest land use and natural vegetation

Potsdam, December 2009

1. Review of Algorithms and Products with Relevance for the EnMAP Toolbox Issue - Geology and Soils

Karl Segl and Hermann Kaufmann



1.1. Geology

1.1.1. Introduction/Basics

Every material especially minerals in rocks and soils are formed by chemical bonds, and as such can be characterised by spectral absorption features in the electromagnetic spectrum. Many of the Earth's materials exhibit significant spectral absorption features in the VNIR and shortwave infrared (SWIR) wavelength regions. These features serve as diagnostic indicators, such as for mineral identification (Hunt and Salisbury, 1970 and 1971; Hunt et al., 1971). Spectral features of rocks and soils originate from electronic and vibrational transitions characteristic of the component minerals. The location of features at definite wavelengths derives from the characteristics of the crystal lattice, such as co-ordination number, nature of ligands and nature of the central ion. Co-ordination number and ligands define the electric field exerted on the central ion and, thereby, the order of magnitude of electronic or vibrational processes. Mineral identification via spectral absorption features is feasible for minerals containing molecules or anions such as H_2O , OH^- , SO_4^{2-} , CO_3^{2-} or CH . This encompasses the phyllosilicates, most sorosilicates, the hydroxides, some sulphates, the amphiboles and the carbonates. Electronic features are caused mainly by charge transfer bands and crystal field transitions of iron in the bi- and trivalent state. In the mineral domain the ferrous and ferric ions dominate the spectral range between 400 nm to about 1200 nm. These ions are widespread in the Earth's surface because of their ability to replace many other ions (e.g., Mg^{2+} , Al^{3+} , Si^{4+} , and Mn^{2+}) in various minerals. Absorption features due to vibrational transitions are located between 1300 nm and 2500 nm, and are caused by overtones and combination tones, originating from the fundamental modes in various multiplicities. These features arise from molecule vibrations or vibrations of atomic groups, which form independent oscillatory units within the molecules. Widely spread oscillatory units in naturally occurring minerals are Al-OH, Mg-OH and C-O. Minerals containing one of these groups show characteristic frequencies within narrow wavelength ranges around 2200 nm (Al-OH) and 2300 nm (Mg-OH/C-O). The exact position of the frequency is determined by the neighbouring molecules or parts of them (Clark, 1993).

This study presents the summary of important applications and up-to-date image analyzing techniques in the fields of geology and soils using hyperspectral data to characterize minerals on the above presented basics that differ considerable from techniques focusing on vegetation targets or water constituents. Recommendations for implementation in the EnMAP toolbox are given in section 1.2.5..

1.1.2. Main Topics in Hyperspectral Remote Sensing Applications and Geology

The main branch of geological research using imaging spectrometry addresses the differentiation of index minerals and the detection and discrimination of minerals and their typical assemblages in hydrothermally altered areas (e.g., propylitic, argillic, sericitic, and potassic). Zonations in such areas, induced by acid solutions percolating on fissures and

cracks, may indicate potential economic ore concentrations. Some typical alteration minerals are kaolinite, dickite, alunite, sericite, chlorite and epidote. All of these can be identified by hyperspectral remote sensing based on their unique spectral signatures.

The same is true for the differentiation of distinct carbonates (calcite, dolomite, and magnesite) whereas dolomitized rocks have a possibility for skarn type mineralization and may serve as oil reservoirs due to increased porosity. The potential of airborne hyperspectral data acquisition for this specific application has been demonstrated by many scientists (e.g., Kruse et al., 1990; Van der Meer, 1994).

Rocks and soils, however, are exposed to various exogenic and endogenic processes that strongly affect their surface characteristics by forming new minerals, weathering crusts and lithobiont communities. Often, exposed rocks and soils are partially covered by sparse vegetation and various kinds of secondary crusts; knowledge about the resulting masking effects on the spectral characteristics of the bedrock/soil is essential for any identification and quantification from hyperspectral data. In addition, internal parameters such as very fine-grained opaque accessory minerals like pyrite, magnetite and graphite, as well as organic compounds quench the spectral signatures of the main constituents that are present (Geerken and Kaufmann, 1989).

Under heavy vegetation conditions, hyperspectral remote sensing from space provide an opportunity to investigate the potential for the detection of mineral deposits by measuring the chlorophyll concentration in the vegetation. Vast areas in the Northern Hemisphere such as boreal and tundra regions are considered to have large mineral occurrences. Geochemical influences such as heavy metal stress (Collins, et al., 1983) and decontaminating methane in extensive, homogeneous vegetation canopies can also be an indication of mineral or oil occurrences.

Abandoned mines and acid mine drainage that affect human drinking water supplies are a major current problem. Many mines and mining districts have been abandoned throughout the world in the past century when mining operations ceased to be economical. Often, there was no consideration of future environmental impacts, nor rehabilitation of such sites. Environmental problems include acidic and metal-rich drainage and leakage of cyanide-bearing solutions.

Imaging spectrometry has been used to map minerals typically generated in arid environments (e.g., gypsum) and to guide remediation efforts, saving millions of dollars. Thus, a major scientific objective is to monitor and characterise these numerous hazardous sites, with special emphasis on the assessment of impacts on the vegetation cover and nearby water bodies.

Applications focusing on tectonic issues are not considered here, as those are approached mainly by highly resolving panchromatic data and InSAR techniques.

Hydrothermal Alterations

Hydrothermal alteration is associated with intrusive or extrusive bodies that initiate the physiochemical interaction of magmatic or meteoric fluids with the surrounding rock. Circulating fluids change the mineralogy of the country rock and form zones with diagnostic mineral assemblages.

The detection of alteration zones that are associated with most hydrothermal ore deposits plays an important role in mineral exploration because the changed mineralogy and texture of the enclosing wall-rock are usually much more extensive and obvious than the ore deposit itself.

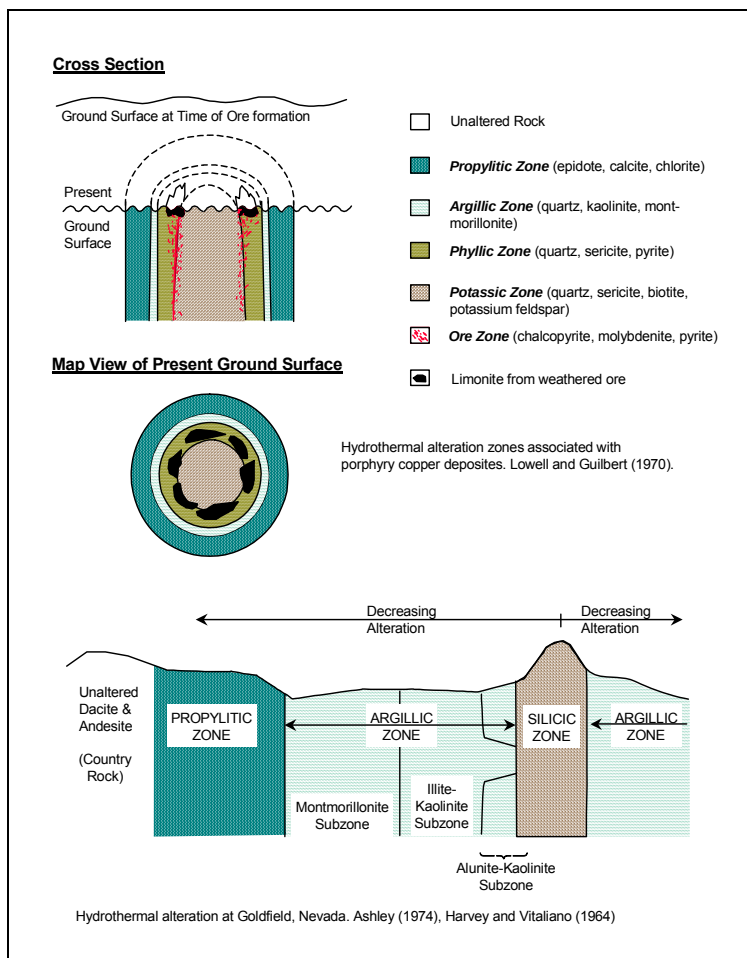


Figure 1: Model of hydrothermal alteration adapted from Sabins(1997) adapted from Sabins (1997).

Hydrothermal alteration forms a visible guide to hydrothermal activity and can be used to locate ore deposits. It usually results in the formation of different zones with a characteristic mineral content (Fig.2). These zones typically show roughly concentric patterns around the ore body and are characterised by different alteration stages of plagioclase. A typical alteration of aluminosilicate rocks shows the following alteration sequence from distant to proximate: a propylitic zone with epidote and/or chlorite; an intermediate argillic zone with kaolinite and montmorillonite; an advanced argillic zone with dickite, kaolinite, pyrophyllite, diaspore, alunite, or other aluminum-rich phases; a sericitic zone with all feldspars altered to sericite; and a potassic zone with potassium-feldspar and/or biotite (Rose and Burt, 1979).

Since most of these alteration minerals show unique absorption features within the VNIR and/or SWIR parts of the electromagnetic spectrum, imaging spectroscopy can be employed to detect these alteration zones.

Gold-bearing Hydrothermal Deposits

The rare occurrence of mineral-bound ammonium has been recognized to often be associated with gold-bearing hydrothermal deposits. Therefore, the presence of mineral-bound ammonium could be used as an indicator element in exploration for gold and other minerals. Unfortunately, a conventional approach is hampered by the fact that a visual differentiation between ammonium-bearing and other hydrothermally altered rocks in the field is impossible. Ammonium is, in contrast to the poor visual distinction, an extremely well suited target for imaging spectrometry, since it shows very distinctive absorption features in the infrared wavelengths between 2.0µm and 2.5µm. Ammonium-bearing minerals include buddingtonite, ammonium-alunite, ammonium-jarosite, and ammonium-illite.

Not only is it possible to map the extent of ammonium-bearing rocks, but the depth of the buddingtonite absorption band at 2.12µm can also be used as a close approximation of the percentage of the contained ammonium when fairly pure buddingtonite is present (Baugh et al., 1998). This is possible due to the linear relationship that exists between the buddingtonite absorption feature at 2.12µm and the ammonium concentration. This method could also be used for other minerals like jarosite, alunite or kaolinite.

Porphyry Coppers

The term porphyry copper deposit refers to large, intrusion-related deposits that contain relatively low grade ores. The main products from porphyry copper deposits are copper and gold or copper and molybdenum. The deposits are found either in or next to intrusive rocks that show a porphyritic texture. Porphyry copper deposits occur within a wide variety of host rocks but coincide worldwide with orogenic belts. Therefore, a great majority of the porphyry copper deposits are found in the circum-Pacific area. Already in the late 1970s, early experiments have been conducted in using remote sensing derived products to aid the exploration of porphyry copper deposits (Abrahams and Brown, 1985).

Porphyry copper deposits generally show the following alteration zones with their associated minerals: a propylitic zone that contains chlorite, epidote, and calcite; an argillic zone that is characterised by clay minerals, montmorillonite, pyrite, and chlorite; a phyllic zone with quartz, sericite and an abundance of pyrite; and, in the centre, a potassic zone that contains biotite, orthoclase, and quartz. In prospecting for porphyry copper deposits, iron oxides and hydrous minerals are key elements for the detection of alteration zones. Since iron oxides have unique absorption features around 1µm and hydrous minerals around 2µm - 2.5µm, these alteration zones can be mapped reliably using spectrometry.

Differentiation of Metamorphic Processes

The study of metamorphism is usually based on mapping the spatial distribution of metamorphic minerals as well as their distribution and abundance within their respective metamorphic zones or various isogrades (e.g., blueschist-, greenschist-, amphibolite-facies). The level of accuracy with which these aspects can be determined is of great importance. Unfortunately, field recognition of most metamorphic minerals is difficult and some crucial ratios of minerals can only be determined by laboratory methods. Near-infrared reflectance spectroscopy could prove to be a very useful and time saving tool for research in metamorphism because most of the key metamorphic minerals show unique spectral absorption features. Recent studies (e.g., Duke and Kozak, 2000) have demonstrated the great potential to map the distribution and abundance of key metamorphic minerals like brucite, serpentine, calcite, tremolite, chlorite and dolomite using imaging spectrometry.

Skarns

Skarn deposits are mined for many important metals, including copper, zinc, iron, and gold, just to name a few. These deposits can form during regional or contact metamorphism and from a variety of metasomatic processes involving fluids of magmatic, metamorphic, meteoric, and/or marine origin. They occur as a replacement deposit in limestone or dolomite and are often found in conjunction with porphyry copper deposits.

Because most skarn deposits are zoned, recognition of alteration features is very important in the early exploration stages. The skarn mineralogy can be mapped using spectrometry and the resulting mineral maps that outline different alteration zones can be used to locate the potential ore body.

Skarns that replace dolomite tend to be magnesian and are usually mined for magnetite. Magnesian skarns contain forsterite, magnetite, and anhydrite. Skarns replacing limestone are more calcic and are commonly mined for tungsten or copper, but in exceptions also for molybdenum, zinc or lead. These calcic skarns contain andraditic garnet, interstitial calcite, bornite and chalcopyrite (Rose and Burt 1979).

Kimberlites (Diamonds)

Kimberlites are a group of volatile (CO₂) rich, potassic, ultrabasic rocks with megacrysts of a variable composition in a fine grained groundmass. These megacrysts can contain ilmenite, pyrope garnet, olivine clinopyroxene, phlogopite, enstatite and chromite. The groundmass or matrix can contain olivine, phlogopite, perovskite, spinel and diopside. Kimberlites occur as clusters of pipes, probably along major crustal fracture zones.

Kimberlite diatremes are roughly circular with a pipe-like or cone shape. Three textural genetic groups of kimberlites are recognized: 1) crater facies (may have high concentrations of diamonds, but are not well preserved), 2) diatreme or tuffisitic facies (volcanoclastic breccias), which are the dominant phase and 3) hypabyssal facies, which may be the best characterised petrographically, although they are poor diamond sources (Kjardgaard, 1995). Alteration of these pipes can be used as a major guide for exploration. The ultramafic minerals associated with kimberlite pipes are highly susceptible to weathering and fluid flow is not restricted in the breccia environment. Olivine in groundmass or crystals will alter to serpentine and this will show detectable compositional changes.

The main types of alteration are serpentinisation, calcification and chloritisation. At the surface, kimberlite weathers to a soft, oxidized rock, "yellow ground", which grades into "blue ground", towards the source or into the pipe. This effect occurs mainly vertically but can also form haloes around a pipe. The yellow colour is due to the oxidation process of olivine to serpentine, to saponite and smectite. Exploration methods for kimberlites include remote sensing methods, in addition to geophysical and geochemical surveys, to identify indicator minerals.

The most common alteration minerals associated with kimberlites are serpentine, calcite, magnesite, phlogopite, biotite, chamesite, clinocllore, saponite, Mg-silicate, vermiculite, and amphibole. Serpentine is one of the most common and diagnostic alteration minerals associated with kimberlites. It shows compositional variations that can be contoured.

Chlorite is also a common mineral associated with kimberlites and can be a product of weathering of serpentines. Chlorites will form alteration haloes around the kimberlite pipes. Vermiculite is a weathering product of chlorite. Fe/Mg micas are sometimes found in high abundance in kimberlite pipes.

Differentiation of Pyroclastic Deposits

Volcanic tephras can form by magmatic fragmentation, the disruption of magmas by internal volatiles, or by hydromagmatism, the explosive interaction of magma with external water. The nature of the resulting tephras provides clues as to which fragmentation was dominant and, if the latter process was responsible, about the amount of external water present at the time of eruption.

Basaltic hydrovolcanism produces a continuum of volcanic landforms. While the most prominent examples are the tuff rings and tuff cones produced by Surtseyan activity, even Strombolian edifices such as cinder cones can have phreatomagmatic episodes. Indeed, the oxidized cinders which are common at many cinder cones are probably the result of some small level of water/magma interaction.

Initially basaltic tephras are characterized by a very low overall reflectance. As basaltic tephras alter, their visual and near infrared reflectance also changes. The alteration of cinders takes the form of the development of well crystalline ferric oxide minerals, principally hematite, which have easily recognizable reflectance spectra. The process by which these cinders become oxidized has never been examined in any detail; however, it seems likely that the most oxidized cinders result from relatively high levels of interaction with water, either internal or external to the melt.

A combination of hydration and oxidation of the sideromelane in tuff cones produce the mineraloid palagonite. Palagonite tuffs, such as those from Easy Chair Crater and the cone portion of Pavant Butte, contain zeolites, poorly-crystalline smectite clays and ferric oxides. These components combine to produce reflectance Spectra that are brighter and spectrally distinct from the tephras typically found in tuff rings.

With increasing oxidation there is a decrease in the center and depth of the "1- μm " band in laboratory spectra of tuff ring and tuff cone samples (Farrand and Singer, 1991). The laboratory spectra indicate that even as Fe^{3+} becomes more important, i.e. in the palagonite tuff samples, there is no development of a resolvable band at 0.86 or 0.9 μm which could be attributed to well-crystalline hematite or goethite. Instead absorption from ferrous and ferric phases seem to be contributing to one composite feature.

Near infrared spectrometry has also proven very effective in detecting poorly crystalline clay minerals in bulk samples of palagonite tuff. Absorptions at 2.2 μm in several tuff ring samples and at 2.3 μm in many tuff cone samples respectively indicate the presence of Al-OH and Mg-OH bearing clay structures.

In the reflectance spectra of silicic tephros, there is a trend which is in many respects opposite to that seen in the basaltic tephros. While basaltic tephros grow brighter with increasing alteration, silicic tephros grow darker with increasing devitrification (Levine, 1989).

Mineral Exploration Based on Vegetation Anomalies

In many cases, direct detection of alteration zones is hampered by the presence of a dense vegetation cover. The presence of vegetation and, in cases, deep weathering of the bedrock often act as a major obstacle for general geologic mapping and mineral resource assessment. Spectroscopy can offer an indirect approach to map the presence of heavy metals or zones of altered lithology in these problematic areas by analysing the spectral reflectance characteristics of the vegetation coverage. This approach is only possible because heavy metals and alterations usually show effects on the pigments of vegetation that are spectrally detectable.

Alterations

If the altered rock is poorer in nutrients than the original rock, this lack of nutrients can lead to a change in species. In this case, the chlorophyll absorption can often be used to successfully discriminate different vegetation types.

Poorer substrate can also result in a sparser canopy that can be detected by spectroscopical means as shown by Rowan et al. (2000), who mapped the distribution of alteration zones in the Carolina slate belt using differences in spectral reflectance of chestnut oak canopies. The distinction was mainly based on the less prominent O-H absorption bands at 0.97 μm and 1.19 μm for the canopy growing on intensively altered bedrock. Their results showed a high accuracy regarding the distinction between vegetation growing on altered vs. unaltered bedrock. The discovery of previously unknown areas with altered rock demonstrates the potential of spectroscopy for mineral prospection.

Heavy Metals and Methane

Accumulation of heavy metals or traces of methane emerging to the surface causes stress on vegetation that manifests in slight damages to the chlorophyll. It can be detected using an airborne biogeophysical technique established by Collins et al. (1983). This technique makes use of the spectral differences that stressed vegetation shows in comparison to healthy vegetation. It uses the shift of the red edge between the absorbance at 0.68 μm by chlorophyll-a and the reflectance plateau due to mesophyll in the near infrared towards shorter wavelengths. The detection of these differences by remote sensing methods requires the high spectral resolution only imaging spectrometers can offer.

Oil and Gas Exploration

In petroleum exploration, imaging spectrometry can be used to detect microseepage. The term microseepage stands for light hydrocarbons that are seeping to the surface. They can be detected at the surface as an alteration in mineral content of the lithology or indirectly, as a stress factor that they pose on a vegetation cover. Alteration phases usually include carbonates and different clays, all of which can be detected spectrally. Vegetation stress detection (e.g., Yang et al., 1999) is based on the changed spectral expression and can be accomplished by airborne spectrometers using the methods described above. Petroleum exploration uses both of these methods to detect areas with the potential for exploitation.

Environmental Applications

Imaging spectrometry has been used as a tool to aid and complement different issues of environmental monitoring, assessment, and remediation efforts. The process of detecting potential problem sources could be automated and field sampling could be focused on a few locations with a high probability instead of randomly testing the whole site. This approach, where possible, has the potential to optimise the cost- and time-efficiency of environmental projects as different investigations have shown. In the following, two applications have been chosen to demonstrate the capabilities of imaging spectrometry as a tool to identify targets of environmental concern.

Mine waste

In recent times, the issue of remediating inactive metal-mine sites became increasingly important, since oxidation of pyrite at the surface of mine waste is thought to produce acidic water. Acidic water in turn can transport a suite of heavy metals and therefore poses a serious threat to water quality and river ecosystems. There are many inactive metal-mine sites with each one having the potential of hosting sources for acid rock drainage and a survey of these mines seems to be unavoidable. The problem is that whole mine sites have to be probed if no previous information about possible sources is available. The waste rock and tailings might be dispersed over large areas and the identification of locations where acid rock drainage originates is usually a very time consuming and expensive task.

Over the past ten years, many efforts have been made to employ spectrometry for the task of mine site remediation. Improvements in sensor technology made it possible that a task, that could not successfully be accomplished in the late eighties due to poor data quality (Kruse et al., 1989), could become a routine that immensely increased the effectiveness of mine waste detection. The success of the application of imaging spectrometry for mine waste detection has been demonstrated by many different authors, including Swayze et al. (1996 / 1998 / 2000), and Clark et al. (1998).

Research conducted after 1996 is usually based on the findings of Swayze et al. (1996), who describe pyrite oxidation as the primary source of mining-related acidic runoff due to the generation of sulfuric acid (H_2SO_4) through the weathering process of pyrite. Acidic runoff in turn can transport heavy minerals in solution and precipitate them when the pH of the water increases above certain levels. This precipitation of secondary minerals usually forms almost concentric patterns around the source of the acid rock drainage.

The easiest way to map acidic mine waste at metal-mines would be the spectral detection of pyrite. This approach, however, encounters three major obstacles that are due to the nature of pyrite's spectral properties: (1) pyrite has a very low reflectance, (2) its Fe-absorption is saturated and (3) it is mostly coated with secondary minerals.

Although pyrite can't be easily identified using spectrometry, its different Fe-bearing secondary minerals, which have unique spectral properties, can be mapped using remote sensing techniques. Their spectral differences are due to strong absorptions in the 1µm range and for jarosite additionally near 0.42µm and 2.3µm. Different shapes and slightly shifted centres of the absorption bands allow for an exact distinction of these secondary minerals. The oxidation sequence for pyrite is known as jarosite to goethite to hematite. Therefore, accumulations of pyrite at the surface should be found in the neighbourhood of jarosite rather than hematite.

Mineral maps generated for abandoned mine sites usually show the approximately concentric patterns around waste piles as mentioned above (although topography can alter the shape significantly), ranging from jarosite in the centre to a mixed area with jarosite + goethite that is surrounded by a larger goethite zone. Hematite sometimes occurs within the goethite zone or at its outer limits.

Chemical analyses on samples unveiled a strong correlation of the concentration of leachable trace metals and spectrally identified mineral zones, with 10-fold leachability values in the jarosite + goethite zone in comparison to the goethite zone. The spectral approach proved to be far more reliable than the usual approach using XRD to determine bulk mineralogy, which showed only weak correlation to the surface mineralogy resulting from spectral mapping (Swayze et al., 2000).

Another very high correlation exists between the pH and the mineralogical zones, indicating that spectral mapping in comparable settings could be used as a method to indirectly measure mine-waste pH without probing large areas. The pH-ranges in the different spectral zones are very consistent and show in the jarosite zone values from 2.3 - 2.6, 2.9 - 3.5 in the jarosite + goethite zone, and 4.5 - 6.1 in the goethite zone (Swayze et al. 2000).

Although a vegetation cover could change the spectral response patterns of the underlying materials, this issue is of lesser concern since the high acidity mostly prevents vegetation to cover the areas under investigation. This in turn allows the spectral approach to be used independently of climate zones.

One concern is that the minerals at the surface of waste piles and tailings may not reflect the mineral composition at depth. It is possible that un-oxidized sulfides are mantled by a layer of non-acid generating secondary minerals. In such a scenario, spectral analysis will not help to detect the acid-generating capacity of the waste rock and tailings beneath the surface. It is believed, however, that these oxidation rinds will prevent water from penetrating to the sulfides and, in effect, isolate them from the aqueous environment (Swayze et al., 1996).

Swelling clays

Swelling soils containing expanding clays cause enormous damage to buildings and infrastructure every year. Geologists and engineers are usually employed to identify areas containing expanding clays. They conduct extensive engineering tests and use x-ray diffraction (XRD) on soil samples to determine swelling potential and mineralogy. The need for extensive sampling over large areas, necessary to ensure reliability and accuracy of the

results, makes these operations a very time- and cost-intensive task. The capability of imaging spectroscopy to identify minerals in soils or rocks could provide a powerful tool to detect occurrences of certain minerals even in test areas with a large spatial extent. Unique spectral absorption features in the SWIR part ($2.0\mu\text{m} - 2.5\mu\text{m}$) of the electromagnetic spectrum make clay minerals a highly suited target for spectral analysis.

A study by Chabrilat et al. (2002) established the swelling properties of different clay minerals and identified those with a high swelling potential. The generated mineral maps show the ability to spectrally discriminate between clays with different swelling potential using near-infrared reflectance spectroscopy. It even proved to be possible to quantify mixtures of smectite, as the mineral with the highest swelling potential, with other, less swelling clays as illite or kaolinite, using the depth of additional absorption features as a measure. Detected exposures of expansive clays correlated well with field observations and proved to be reliable even in areas where vegetation cover was present.

Summary and Relevance of Applications and Parameters

In this section the effort is made to estimate the relevance of applications and parameters based on a statistical analysis of the reviewed literature.

Applications

Hyperspectral applications with a considerable geological background represent a minority within the reviewed literature. Most papers deal with the description or comparison of new algorithms for improved mineral mapping that use arbitrary spectra from a library without any geological relevance. Nevertheless, some papers were identified leading to following ranking of applications:

1. Hydrothermal alterations (14)
2. Environmental applications (12)
3. Mineral Exploration based on vegetation anomalies (3)
4. Differentiation of metamorphic processes (2)
5. Skarns (1)
6. Kimberlite (1)
7. Differentiation of pyroclastic deposits (1)

Hydrothermal alteration mapping with airborne hyperspectral data was the topic of 14 papers followed by environmental applications dealing with the management of active and abandoned mine regions (12 papers).

Parameters

Parameters that are retrieved from the hyperspectral data with relevance to geological applications are predominantly minerals and rocks. Following minerals were identified in the literature:

Adradite, Alunite, Antarcticite, Antigorite, Biotite, Bischofite, Buddingtonite, Brucite, Calcite, Chalcedony, Chabazite, Chlorite, Cristobalite, Dickite, Dolomite, Dumortierite, Epidote,

Ferrihydrite, Goethite, Gypsum, Halcite, Halloysite, Hectorite, Hematite, Illite, Jarosite, Kaolinite, Limonite, Lepidochrosite, Mesolite, Mica, Mirabilite, Montmorillonite, Muscovite, Neodymion, Nontronite, Paragonite, Peridotite, Pimelite, Pyrite, Pyrope, Pyroxene, Pyrophyllite, Quartz, Saponite, Scapolite, Scolecite, Serpentine, Silicia, Sillimanite, Smectite, Sphene, Talc, Tremolite und Zeolite.

To rank their relevance in the reviewed literature the statistical occurrence of single minerals was counted. The result is depicted in Fig.. 2:

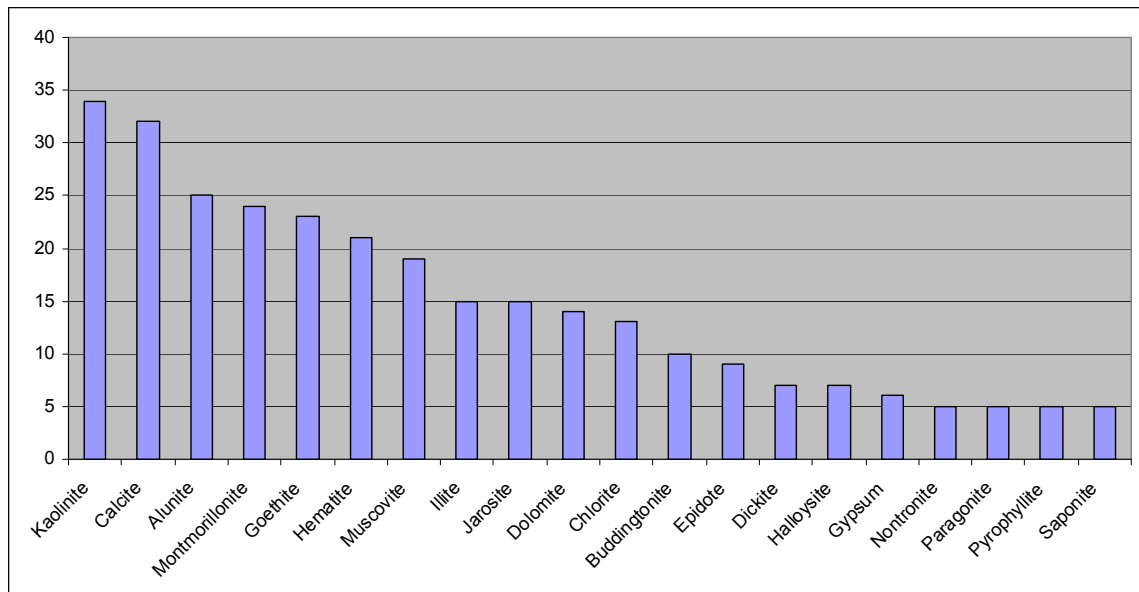


Figure 2: Statistical occurrence of minerals

Kaolinite is the most common used mineral followed by calcite, alunite, montmorillonite, goethite, etc.. Clay minerals, Carbonates and iron oxide.

Beside the dominating minerals some rock types were also classified such Andesite, Bentonite, Granadiorite, Granite, Metatonalites, Metagabbro, Monzogranites, Monzonite, Palagranite, Psammites'und Rhyolite as well as vegetation stress parameters.

1.1.3. Parameter Retrieval Strategies

The previous chapter showed that mineral types are the key parameters that must be retrieved from hyperspectral imagery. There exists a whole bunch of algorithms for this problem in literature that can be classified into three groups - algorithms that support the ENVI-processing scheme, expert systems and empirical regression techniques. The retrieval of vegetation stress parameters is excluded from this investigation since it is one of the main topics in the review study by Heike Bach.

ENVI-Processing-Scheme

The typical ENVI-Processing scheme consists of three major steps (Kruse, 1998). The basic concept is to reduce the data to manageable levels by finding those pixels in the image that can explain every other pixel in terms of a mixing model. It starts with the Maximum-Noise-Fraction Transformation (MNF) of the reflectance imagery reducing the spectral dimensionality of the data by finding linear combinations of bands that explain the inherent dimensionality of the data. The second step the dimensionality is further reduce by finding key endmembers. For this purpose ENVI offers the Pixel Purity Method combined with the n-D Visualizer. Once endmember spectra have been extracted, they have to be identified. In a third step these identified image endmembers are then used to extend the analysis back to the full spatial/spectral dataset to produce image maps showing the location and abundance of specific materials (inversion process).

There hardly exist significant options to the standard MNF-Transformation (step 1) for a meaningful reduction of the dimensionality of the feature space in the literature, however, many algorithms address the automated endmember determination (step 2) and the inversion process (step 3). Up-date-algorithms from both fields are described in the following:

Algorithms for Image-Based Endmember Detection

Endmembers determination is very important in hyperspectral data analysis. It is the process to find pure signatures present in image data, which are generally of major interest for image analysis. Several approaches such as Pixel-Purity-Index, N-FINDR, Convex Cone Analysis, Vertex Component Analysis etc. have exploited geometric features of hyperspectral mixtures to determine the smallest simplex containing the data. Those geometrical based methods assume the presence in the data of at least one spectrally pure pixel of each endmember defined by the vertices of the simplex. However, this requisite may not hold for all data sets. Hence, a second group of approach such as Iterative Constrained Endmembers, Independent Component Analysis, Dependent Component Analysis, etc. was developed that don't need to have spectrally pure pixels in the observations. Other techniques like the Dependent Component Analysis (DECA) and Constrained Positive Matrix Factorization (CPMF) optimize endmember detection and unmixing within a single processing step. In the following a summary of the most prominent methods is presented:

Pixel Purity Index (PPI)

The PPI algorithm is a well known approach used in endmember determination (Boardman et al., 1995). PPI finds the most spectrally pure pixels in the image by repeatedly projecting an n-dimensional scatter plot onto random unit vectors comprising the MNF-transformed data. The extreme pixels in each projection are recorded and the total number of times each pixel is marked as extreme is noted. Those Pixels marked as extreme above a certain threshold are declared "pure". To exclude the redundant spectra in the pure pixel list, the actual endmember spectra are selected by a combination of intelligent review of the spectra themselves and through N-dimensional visualization. This tool is included in the ENVI software.

Iterative Error Analysis (IEA)

In the IEA algorithm, a series of constrained unmixing operations is performed, each time selecting as endmembers the pixels that minimize the remaining error in the unmixed image (Neville et al., 1999). An initial vector (usually the mean spectrum of the data) is chosen to start the process. A constrained linear spectral unmixing in terms of this vector is performed, and the error image, formed by the errors remaining at each pixel after the unmixing operation, is calculated. The user then selects a desired number of endmembers E , a number of pixels R , and an angle value θ . R is the number of pixels with the largest number of errors, selected from the error image. The spectral vector corresponding to the pixel with the single largest error is found. A subset of R consisting of all those pixels that fall within an angle θ of the maximum error vector is then calculated, and these pixels are averaged to produce the new endmember vector. This process is continued until E endmembers have been selected.

N-FINDR

N-FINDR attempts to find the simplex of maximum volume that can be inscribed within the hyperspectral data set using a simple non-linear inversion (Winter, 1999a). The non-linear inversion procedure begins with a random set of pixels as endmembers. In order to refine the estimate of endmembers, every pixel in the image must be evaluated as to its likelihood of being a pure or nearly pure pixel. To do this, the volume must be calculated with each pixel in place of each endmember. A trial volume is calculated for every pixel in each endmember position by replacing that endmember and recalculating the volume. If the replacement results in an increase in volume, the pixel replaces the endmember. This is repeated until there are no more replacements.

Optical Real-time Adaptive Spectral Identification System (ORASIS)

This method has been under development at the Naval Research Laboratory (NRL). This algorithm does not do dimensionality reduction; instead it thins the data set using Exemplar Selection process in which any redundant spectra are rejected. The rejection is done by calculating the angle between spectral vectors; vectors that are not separated by a threshold angle are thinned from the data. The algorithm then finds a basis set of much lower dimension, than the original data using Gram-Schmidt orthogonalization. The thinned data are then projected onto this basis subspace and a simplex is found through a minimum volume transform.

Automated Morphological Endmember Extraction (AMEE)

The input to the AMEE method is the full image data cube, with no previous dimensionality reduction (Plaza et al., 2002). The method is based on two parameters: a minimum and a maximum spatial kernel size. First, a minimum kernel is considered. This element is moved through all the pixels of the image, defining a spatial context around each hyperspectral pixel. The spectrally purest and the spectrally most highly mixed spectral signatures are respectively obtained at the neighborhood using two basic morphological operations. A morphological eccentricity index (MEI) is then obtained by calculating the spectral angle distance between the two signatures. This operation is repeated for all the pixels in the scene, using kernels of progressively increased size, and the resulting scores are used to evaluate each pixel in both spatial and spectral terms. The algorithm performs as many iterations as needed. The associated MEI value of selected pixels at subsequent iterations is

updated by means of newly obtained values, as a larger spatial context is considered, until a final MEI image is generated. Endmember selection is performed by a fully automated approach consisting of two steps: 1) autonomous segmentation of the MEI image, and 2) spatial/spectral growing of resulting regions.

Iterative Constrained Endmembers (ICE)

The ICE has a more statistical nature. It combines ideas from convex geometry and multivariate curve resolution techniques to find endmembers, which trades off goodness-of fit of the convex geometry model against the size of the simplex (Berman et al., 2003).

Convex Cone Analysis (CCA)

This method is based on the fact that physical quantities, such as radiance and reflectance, are nonnegative. The vectors formed by discrete radiance/reflectance spectra can be expressed as linear combinations of nonnegative components, which lie inside a nonnegative, convex region. The objective of CCA is to find the boundary points for that region. To implement this concept, the method finds the eigenvectors of the sample spectral correlation matrix of the image, and selects those eigenvectors corresponding to the E largest eigenvalues (where E is the *a priori* number of endmembers to model). The method then looks for the boundaries of the convex cone, where the linear combinations of these eigenvectors produce vectors that are strictly nonnegative. These identified corners of the convex cone represent the endmembers.

Vertex Component Analysis (VCA)

The VCA algorithm (Nascimento, 2005) is based on the geometry of convex sets. It exploits the fact that endmembers occupy the vertices of a simplex. VCA algorithm assumes the presence of spectrally pure pixels in the data and iteratively projects data onto the direction orthogonal to the subspace spanned by the endmembers already determined. The new endmember signature corresponds to the extreme of the projection. The algorithm iterates until the number of endmembers is exhausted.

Independent Component Analysis (ICA)

Independent component analysis (Hyvärinen and Oja, 2000) is an unsupervised source separation process that has shown success in blind source separation, feature extraction, and unsupervised recognition (Chang et al., 2002). Unlike the Principle Component Analysis, the ICA looks for components which are statistically independent rather than uncorrelated. Thus, it requires statistics of orders higher than second order. The idea of the ICA makes use of a linear model to describe a mixture of a set of unknown random signal sources, then demixes them in separate components so as to achieve signal detection and classification. Finding a linear decomposition of data into statistically independent components, this technique enables the definition of meaningful endmember spectra from data where pure pixels are not present. However, the dependence on mutually independent sources, which is not the case of hyperspectral data, since the sum of abundances fractions is constant and additionally noise degrade the ICA performance.

Independent Factor Analysis (IFA)

Independent factor analysis (Attias, 1999) was introduced as a method for recovering independent hidden sources from their observed noisy mixtures. IFA is divided into two steps. First, source densities and noise covariance are estimated from the observed data by maximum likelihood. Second, sources are reconstructed by an optimal nonlinear estimator. Although IFA is a well suited technique to unmix independent sources under noisy observations, the dependence among abundance fractions in hyperspectral imagery comprises, as in the ICA case, the IFA performance.

Dependent Component Analysis (DECA)

This method decomposes a hyperspectral image into a collection of endmember spectra of materials present in the scene and the corresponding abundance fractions at each pixel (Nascimento and Bioucas-Dias, 2007). DECA assumes that each pixel is a linear mixture of the endmembers signatures weighted by the corresponding abundance fractions. These abundances are modelled as mixtures of Dirichlet densities, thus enforcing the constraints on abundance fractions imposed by the acquisition process, namely non-negativity and constant sum. The mixing matrix is inferred by a generalized expectation-maximization (GEM) type algorithm. This method overcomes the limitations of unmixing methods based on ICA and on geometrical based approaches.

Constrained Positive Matrix Factorization (CPMF)

This approach deals with the unsupervised determination of the constituents and the fractional abundance in each pixel of a hyperspectral image using the constrained positive matrix factorisation (Masalmah, 2007). This algorithm consists of three different steps: determination of number of endmembers, initialization, and computing the constrained positive matrix factorisation. The positive rank the image matrix is used as the starting number of endmembers and the SVD-subset selection approach for the initializing of the algorithm. After this, the computation of CPMF is done using the Gauss-Seidel algorithm.

Algorithms for Mineral Classification and Spectral Unmixing

The third step of the ENVI-processing scheme is the inversion process. The techniques can be classified into three major approaches:

Target Signature-Constrained Pixel Detection representing the typical classification techniques such as Spectral Angle Mapper (SAM), Spectral Feature Fitting (SFF), etc.

Target Abundance-Constrained Subpixel Detection

Including full spectral unmixing techniques such as Linear Spectral Unmixing (LSU) and Non-Negative Least-Squares Estimation (NNLS) as well as partially spectral unmixing techniques like Orthogonal Subspace Projection (OSP).

Target Signature-Constrained Subpixel Detection

Representatives are matched filters based detectors. Similar to partial unmixing, they are used to minimize the output of undesired signatures to further improve the target discrimination performance. Representatives are e.g. Matched Filtering (MF), Mixture Tuned Matched Filtering (MTMF) or Constraint Energy Minimization (CEM).

Spectral Angle Mapper (SAM)

The algorithm uses the n-dimensional angle to match pixels with reference spectra (Kruse et al., 1993). The spectral similarity is defined by the angle between two spectra, treating them as vectors in a space with dimensionality equal to the number of bands. Using reflectance data, the technique is insensitive to illumination and albedo effects. The algorithm compares the spectral shape characteristics of pixels that include absorption features as well as continuum information. Both are weighted equally which can lead to misclassifications. This tool is included in the ENVI software.

Spectral Feature Fitting (SFF)

This technique concentrates only on absorption features (Clark et al., 1990). Therefore, a continuum removal from the image and reference data set is applied a priori. The image spectrum is modelled by applying a scaling factor on the reference spectra. This factor is estimated by least-squares estimation. The achieved RMS-error represents a measure for spectral similarity. The technique produces reasonable results for spectra with clear absorption characteristics. This tool is included in the ENVI software.

Multiple Spectral Feature Mapping (MSFM)

The Multiple Spectral Feature Mapping Algorithm (MSFMA) was developed by Clark et al. (1991). This technique uses least-squares fitting between a scaled laboratory reference spectrum and hyperspectral reflectance data for each pixel. Multiple spectral features can be fitted for each mineral and an unlimited number of minerals can be mapped simultaneously. Quality of fit and depth from continuum numbers for each mineral are calculated for each pixel and the results displayed as a multicolor image.

Spectral Identification Method (SIM)

The Spectral Identification Method supplies estimates according to confidence levels of the existence or not of the curve sought (Carvalho et al., 2001). The method is based on two procedures: the algorithm of similarity of the SIM spectral classifier and the ANOVA statistical method. This method generates an image of the similarity parameter as much from the SIM as from three relative binary images of the existence of the material according to confidence levels.

Multilayer Perceptron (MLP)

Artificial neural networks represent parallel computational models comprised of densely interconnected adaptive processing units. A very important feature of these networks is their adaptive nature, where "learning by example" replaces "programming" in solving problems. This feature makes such computational models very appealing in application domains where the analyst has little or incomplete understanding of the problem to be solved, but where training data are readily available. For classification purposes, feed-forward network types such as Multilayer-Perceptron (MLP) is used. The MLP allows an universal function approximation since they represent highly complex, non-linear regression models. The parameters of the model are estimated by linear and non-linear optimisation techniques based on training samples. Due to the high flexibility of these models, user experience is required for network design and parameter estimation. An example for mineral classification is presented in (Segl et al. (1994). A continuum removal is applied a priori to support the

algorithm for finding an appropriate solution based only on absorption features. The trained network is able to identify numerous, even similar minerals based on smaller variations within the absorption bands and different feature combinations. However, the extracted decision rules are not forthcoming due to the black box character of the networks. Therefore, the trained network may describe only local properties of the test site limiting the applicability to other test sites. This tool is included in the ENVI software.

Linear Spectral Unmixing (LSU)

The basic assumption on which linear spectral unmixing (or also referred as Spectral Mixture Analysis (SMA)) is based is that the spectrum of a mixed pixel has been created by the linear superposition of the spectra of the pure components called endmembers, and the coefficients of the linear superposition are equal to the fractional coverages of the field of view of the pixel by the corresponding endmembers. This technique belongs to the group of full unmixing algorithms requiring the knowledge of all endmember spectra in the dataset. Their fractional abundances are retrieved by least-squares or constrained least-squares estimation assuming that the sum of all abundances is 100%. An important drawback of this technique is that negative abundance values cannot be excluded in the estimation process. This tool is included in the ENVI software.

Non-Negative Least-Squares Estimation (NNLS)

The NNLS algorithm is based on the same linear spectral mixture model as the LSU. It solves the system of equations in a least squares sense, subject to the constraint that the solution vector (abundances) has non-negative elements.

Multiple Endmember Spectral Mixture Analysis (MESMA)

Another source of error of the LSU is that it considers the pixels as a mixture of all endmembers also it is very likely that most of them are absent. To correct this kind of error the MESMA algorithm allows the variation of the number and quantity of endmembers pixel by pixel in the image (Roberts et al., 1998). The algorithm adopts as the best model the one that has smaller root mean square error when compared to the spectral curve of the pixel. The computational effort is a problem as the possible combinations increase with the number of endmembers.

Semi-Parametric Unmixing (SPU)

The semi-parametric unmixing is based on a combined linear and additive model with a non-linear, smooth function to represent end-member spectra unaccounted (Nielsen, 2001).

Hierarchical Bayesian Model (HBM)

The hierarchical Bayes Model is one of the most important topics in modern Bayesian analysis. It is a powerful tool for expressing rich statistical models that more fully reflect a given problem than a simpler model could. This technique can be adapted to estimate the fractional abundances of endmembers assuming a linear mixture of spectra (Dobigeon and Tournet, 2007). Appropriate priors must be introduced to guaranty the positivity and additivity constraints inherent to the mixture fractions. These coefficients are then estimated from their posterior following the principles of Bayesian inference. The estimation is performed by using a Gibbs sampling strategy generating samples distributed according the

abundance posteriori distribution. These samples are then averaged yielding the abundance minimum mean square error estimator.

Orthogonal Subspace Projection (OSP)

OSP belongs to the group of partial unmixing algorithm (Harsanyi and Chang, 1994) splitting the linear mixture model into two terms, one describing the known endmembers and their abundances and one consisting of undesired or often unknown endmembers. The idea of OSP is to project the observations onto a subspace orthogonal to the background space defined by these undesired endmembers. However, this requires the knowledge of both endmember groups. Nevertheless OSP can be used to remove the effect of known spectra. There exists many extended versions of the OSP approach that include improvements like the Oblique Subspace projection classifier (OBC), Signal Space orthogonal Projection classifier (SSC) and Target Signature Space orthogonal Projection classifier (TSC) (Chang et al., 1998).

Constraint Energy Minimization (CEM)

CEM maps targets from their spectral characteristics without knowing the spectral characteristics of the background endmember. The match filtering minimizes the variance of the overall spectral response and gives unit scores only to perfect matches. The pixels that exist in sufficient quantity and with sufficient spectral contrast are the covariance drivers of the image statistics. Those spectra will be properly nulled and receive a near-zero filter response. Pixels that have a significant contrast but only exist in limited quantity will not be properly nulled and will be mapped as false positives.

Matched Filtering (MT)

Another traditional method used for classification is the processing of data using a matched filter based on a target spectrum of interest. Similar to OSP and CEM matched filtering is used to maximize the signal of a known endmember and to suppress signals of the composite unknown background, thus "matching" the known signature (Chen and Reed, 1987). This is accomplished by defining a "spectral prototype" (endmember) and, on a pixel-by-pixel basis, computation of the cross-correlation between the spectral prototype and the image spectra. The results of matched filtering are presented as grey-scale images with a value range from 0 to 1.0, with 1.0 being a perfect match and 0 showing no correlation.

Matched filtering offers a quick method of detecting specific minerals based on matches to a specific library or image endmember spectra. Although the results are similar to those produced with spectral unmixing, it requires significantly less computation. One of the problems using the matched filter technique arises when mixed pixels are present in the scene. This situation causes a mixture of spectral signatures for the pixel and a match with the signature of a spectrally pure endmember would require a rather low threshold that, in turn, leads to misclassifications. This tool is included in the ENVI software.

Mixture Tuned Matched Filtering (MTMF)

MTMF combines the best parts of the Linear Spectral Mixing model and the statistical Matched Filter model while avoiding the drawbacks of each parent method. From Matched Filtering it inherits the advantage of its ability to map a single known target without knowing the other background endmember signatures, unlike traditional Spectra Mixture modeling.

From Spectral Mixture modelling it inherits the leverage arising from the mixed pixel model, the constraints on feasibility including the unit-sum and positivity requirements, unlike the Matched Filter which does not employ these fundamental facts. As a result MTMF can outperform either method, especially in cases of subtle, sub-pixel occurrences. This tool is included in the ENVI software.

Target Constrained Interference Minimized Filter (TCIMF)

This approach takes advantage of the strengths of the CEM while improving its disadvantages. It divides targets of interest into a class of desired targets and another class of undesired targets while considering interference as a separate signal source (Ren and Chang, 2000). With this 3-component signal source model, the TCIMF can be designed to achieve detection of desired targets, annihilation of undesired targets and minimization of interfering effects all together in one operation. It improves the CEM in the sense of the effects of undesired targets being minimized rather than being eliminated.

Expert Systems

Many naturally occurring materials can be identified and characterized based on their unique spectral characteristics. In geology, the exact position and shapes of diagnostic absorption bands are different for different minerals in the visible and near infrared region (0.4 – 2.5µm) of the spectrum allowing their direct identification. This knowledge can be used to build up an expert system for automated mineral identification. Besides a first in-house expert system built by NASA experts (Chiou, 1985), only two scientific groups around Clark and Kruse met this challenge.

Expert System from Kruse

Kruse et al., 1993 developed an expert system that allows automated identification of Earth surface materials based on their spectral characteristics in imaging spectrometer data. Automated, techniques were developed for the extraction and characterization of absorption features by analyzing a suite of laboratory spectra of some of the most common minerals (25 samples). Critical absorption band characteristics for identification were defined, and these were used to develop facts and rules defining a generalized knowledge base for analysis of reflectance spectra that allowed the computer to make decisions similar to those that would be made by an experienced analyst. The expert system produced image maps from hyperspectral image data showing the predominant surface mineralogy.

Tricorder

The USGS Tricorder algorithm is an expert system which compares the absorption features present in each pixel of hyperspectral data to characteristic absorptions of minerals in the USGS spectral library (Clark et al. 1990a, Clark et al., 1991). The algorithm uses the continuum removal to isolate specific absorptions and remove the effects of changing slopes and overall reflectance levels. Tricorder compares the wavelength position and shape of absorptions with reference spectra. A modified least-squares fitting algorithm is used to assess the closeness of the match. The Tricorder expert system makes further refinements to select the closest match using threshold values, continuum slope constraints and other methods.

Tetracorder

The successor of the Tricorder expert system is the USGS Tetracorder system (Clark et al., 1995). The Tetracorder algorithm compares continuum-removed absorption features of spectra kept in a reference library to those of an observed spectrum. The proper standard library contains spectra of more than 120 materials including minerals, amorphous materials like weathering products, environmental materials like mine waste, vegetation, mineral mixtures, ice and snow, etc.. The algorithm can be trained to compare sets of diagnostic absorption features for a given material according to a set of user-defined rules. The system includes options allowing the user to exclude materials from consideration based on the presence or absence of certain absorption features. Each absorption feature under consideration is normalized against its continuum and then scaled by a multiplicative constant so that its depth matches that of the corresponding reference absorption feature. Least-squares correlation coefficients are calculated and weighted according to the area under the curve and/or optional user-defined weights. Sets of absorption features for specific materials are compared based on a prescribed set of rules. An identification is issued based on application of these rules to the calculated values. For imaging spectroscopy applications, an image is generated for each material under consideration, with the intensity of each pixel corresponding to the product of correlation coefficient and absorption band depth.

Algorithms for Mineral Quantification

Different mineral concentrations cause variations in the depth of the absorption bands. This fact can be used to build empirical models describing the mineral concentration. Field samples are analysed in the laboratory and correlated with the depth of continuum removed spectra (Krüger et al., 1998, Baugh and Kruse, 1998). Besides the depth other features describing the shape of spectra are also possible (Carvalho et al., 2001). After the selection of the regression model describing the best relation between spectral feature and concentration, the model is applied to the hyperspectral image data to create a mineral concentration map. Each pixel is reduced to its spectral feature value and finally transformed to a mineral concentration.

Summary and Relevance of Methods

Many methods have been developed for classification or quantification of mineral abundances during the last decade. A meaningful evaluation of the methods is very difficult. After reviewing the literature, the reader gets the impression that with exception of some papers there exist a negative correlation between the quality of the application and the used methods. This is shown schematically in Fig. 3. Investigations including an excellent geological application are done by geologists and therefore the used methods are limited to easy to use software. In contrast, high advanced mathematical methods are applied by mathematicians and used for the analysis of artificial mixtures of some arbitrary spectra from the USGS library. An accurate evaluation based on a geological application is not interesting for most authors. There exist some exception that realized that an interdisciplinary collaboration is necessary like the groups around Kruse and Clark. In the following the effort is made to compare and evaluate the different approaches.

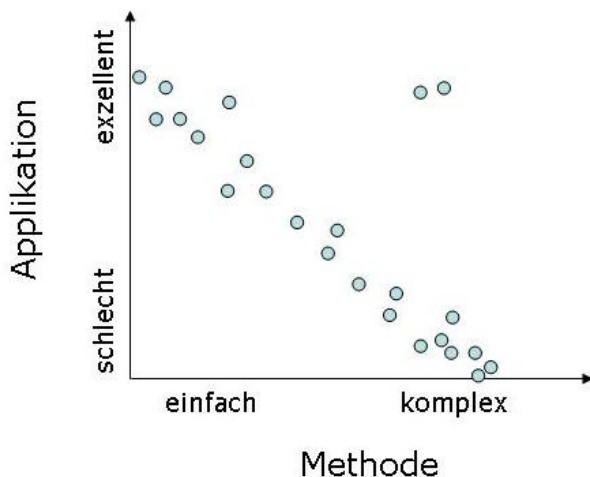


Figure3: Negative correlation between application and method adapted from Sabins (1997).

Endmember Detection Algorithms

The quality of endmember detection is crucial for the accuracy of the final image analysis. The unsupervised approaches as suggested within the ENVI-processing-scheme are convenient, however, may lead to undesired endmember spectra. This becomes in particular true, if the materials of interest are sparsely distributed within the image. In addition, the extracted endmember spectra must be identified. Hence, the potential for automation of the image analysis process is limited.

The presentation of a new algorithm is always linked with the comparison to other techniques. Such a comparison is difficult, because they represent unsupervised techniques extracting different endmembers. Therefore, the evaluation of methods is based on artificial mixtures of up to three mineral spectra stating some benefits for the new technique. Such results cannot be generalized. In fact, this means that there might be a potential for real geological applications but still has to be investigated.

Fig 4. depicts the statistical occurrence of techniques in the reviewed literature. N-FINDR, ICA and PPI are the most common used methods. The high scores of N_FINDR and PPI result from their frequent use as comparison methods.

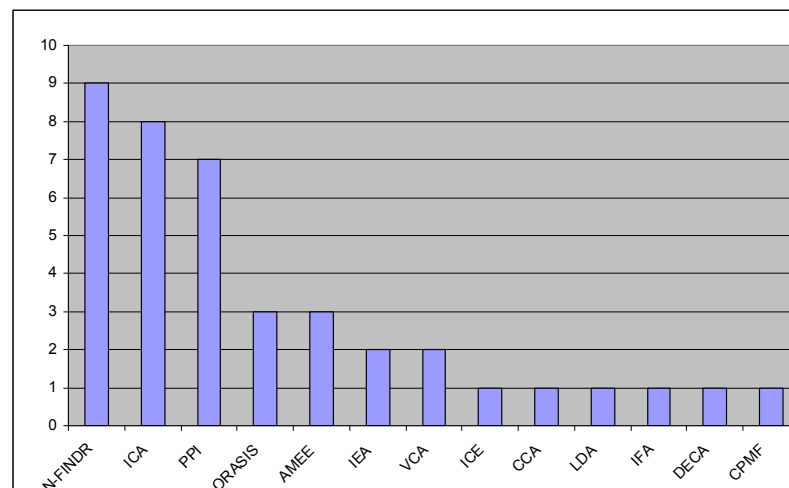


Figure 4: Statistical occurrence of endmember detection algorithms adapted from Sabins (1997).

Inversion Process

Similar to the endmember detection algorithms there exist many investigations including a comparison of classification or unmixing techniques. However, the geological background of all these studies is also limited to the analysis of artificial mixtures of some arbitrary mineral spectra providing only indications for their potential in terms of mineral mapping.

The statistical occurrence of methods is presented in Fig. 5. Most frequent used techniques are LSU, SAM, SFF, MTMF, and MF that are all included in the ENVI-software. Hence, they are easy to use for comparison purpose but also for the analysis of hyperspectral data for people with limited mathematical background.

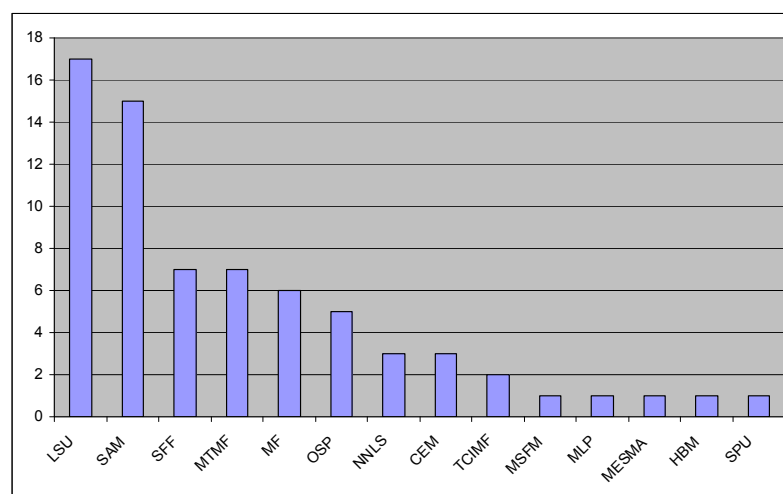


Figure 5: Statistical occurrence inversion algorithms adapted from Sabins (1997).

Expert Systems

The implementation of an expert system requires knowledge from the field of geology as well as from informatics meaning that interdisciplinary teamwork is imperative. Expert systems require less knowledge from the user since the decision process is automated. The most frequent used expert systems in the reviewed literature are the Tricorder followed by its successor the Tetracorder (Fig. 6). These techniques have all shown their great potential for automated mineral mapping in many investigations using AVIRIS data. The latest technique is the Tetracorder that is a public domain software and can be downloaded from the Internet via <http://speclab.cr.usgs.gov/tetracorder.html>. Nevertheless, it is written in FORTRAN including a non-user friendly data input structure.

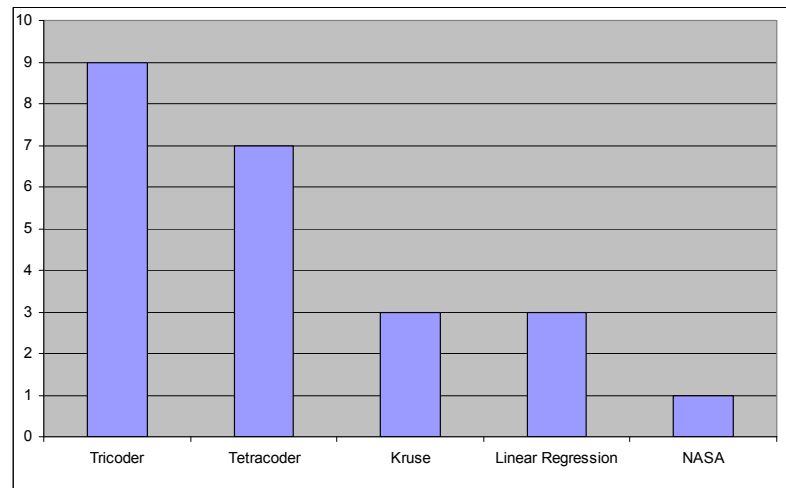


Figure 6: Statistical occurrence of expert systems and quantification algorithms adapted from Sabins (1997).

1.1.4. Priorities and Recommendation for Implementation

A scenario of three different options seems to be feasible for implementation in the EnMAP Toolbox including standard and improved techniques:

ENVI processing scheme

A selection of different endmember detection, classification, spectral unmixing and match filter algorithms that are all not available within commercial software packages can be implemented in the toolbox. This variety allows the user to select the most suitable techniques for the data processing of the respective test site. Most algorithms rely on well known mathematical methods applied now to hyperspectral data. Hence, it is easy for skilled programmers to implement these techniques. These methods can be classified as “nice to have”.

Expert System

The implementation of a new expert system for mineral mapping seems to be the greatest challenge. Especially users that are new to the field of hyperspectral mineral mapping would greatly benefit from such a system. As a first step the tetracoder algorithm can be improved by a user friendly input window structure. Nevertheless, an improved expert system including soft rules (e.g. Fuzzy Logic), latest spectral absorption feature extraction techniques and the possibility to include as much as possible geological and lithological a priori knowledge is highly recommended. Such features are still missing in the current tetracoder algorithm. The design and implementation of such a system is certainly much more complex and time-expensive compared to the first option, however, the benefit significant higher.

Mineral Quantification

The quantification of mineral concentrations is based on simple empirical correlation models. Such models are indispensable tools for the extraction of soil and vegetation parameters. Hence, an explicit recommendation seemed to be of no importance as they have to be available in the toolbox anyway.

Tab.1 includes a summary of the three options including some pros and cons:

Table 1: Recommendation for implementation in the Toolbox

Option	Feature	Pros	Cons	Priority
Expert System	New and more flexible system similar to the Tetracorder including latest technology	High degree of automation; New and unskilled users benefit	Complex and time expensive	1
	Tetracorder including a user friendly data input structure			2
ENVI Processing Scheme	Implementation of several endmember detection and inversion algorithms	Easy to build	Low degree of automation; Experience required	2
Quantification	Empirical correlation models	Covered by vegetation and soil parameter retrieval algorithms		

1.2. Soils

1.2.1. Introduction

This chapter presents the summary of important applications, parameters and up-to-date image analyzing techniques from the field of soils using hyperspectral data. General soil has been defined as “the upper layer of the earth which may be dug, plowed, specifically, the loose surface material of the earth in which plants grow” (Thompson, 1957). Soil is a complex material that is extremely variable in its physical and chemical composition. It is formed from exposed masses of partially weathered rocks and minerals of the earth’s crust. Soil formation or genesis is strongly dependent on the environmental conditions of both the atmosphere and the lithosphere. The soil body is a product of five factors: climate, time, organisms, topography, and parent materials. The great variability in soils is the result of interactions of these factors and their influence on the formation of different soil profiles (Buol et al., 1973). In general, the soil profile, composed of several horizons, typically refers to A (the upper, termed as alluvial horizon), B (the intermediate, termed as illuvial horizon), and C (the lowest, a parent material horizon). The spectral reflectance of soils is a cumulative property that derives from the inherent spectral behaviour of heterogeneous combinations of minerals organic matter and soil water (Irons et al., 1989) of one of the above horizons. Soils in semi-arid regions often have very little organic material and, therefore, almost exclusively consist of rock and mineral particles. An excellent review on image spectrometry for soil applications can be found in Ben Dor et al., 2008.

1.2.2. Main Topics in Hyperspectral Remote Sensing Applications and Soils

Spatial variations of soil characteristics play an important role in determining processes such as loss of vegetation and soil through land degradation and soil erosion processes. Soil erosion is primarily caused by wind and water, soil degradation mainly by desertification, salinisation, acidification, sealing, soil compaction and contamination. All these processes may change different soil parameters such as pH-value, cations exchange capacity, microbiotic activity, infiltration capacity, organic matter content and content of salt.

One of the most important issues of land degradation monitoring is the determination of indicators for degradation processes. It is widely agreed that accelerated erosion is one of the most important sources of soil degradation that, together with the destruction of vegetation cover and structure, contributes to the potential increase of land degradation and desertification. Both are often connected, since the degree of soil degradation is in many ways a reflection of the state of vegetation that covers and conditions it (Perez-Trejo, 1994). Soil salinity is another major cause for soil degradation. This is usually due to rising water tables, either induced by land clearing alone, referred to as dryland salinity, or by irrigation, referred to as irrigation-induced salinity. Spectrally based studies by many researchers (e.g., Ben-Dor, 2002; Metternicht & Zinck, 1997, 2003; Taylor et al., 1994) have shown that detailed spectral information can directly and indirectly pinpoint saline-infected areas. Additionally, quantitative measures of the soil development status form important indicators for the assessment of land degradation/desertification, soil erosion risks, and the mapping of soil degradation severity (Hill, 2000).

Most operational applications of imaging spectroscopy regarding soil contamination have been performed in the context of chronic or accidental pollution resulting from metal mining. Chevrel et al., 2003 investigated six mining areas, five within Europe (Portugal, United Kingdom, Germany, Austria, and Finland) and one in Greenland using HyMap airborne imaging spectrometer data. Imaging spectroscopy was used for mapping the extent and type of chronic contamination with heavy metals using primarily trace minerals of pyrite oxidation as an indirect indicator of potential contamination, which forms an indispensable basis for environmental impact assessment, environmental monitoring of historical mining sites, and remediation planning.

In April 1998, the dam of a mine tailings pond in Aznalcollar (Spain) collapsed and flooded a soil area of more than 4000 ha with pyrite bearing sludge containing high concentrations of heavy metals. Kemper & Sommer, 2002 and 2003 performed a research study combining a field-based chemometric study with the application of HyMap airborne data. It was possible to analyze concentration of heavy metals such as As, Fe, Hg, Pb, S, and Sb with a very high accuracy.

Various important soil characteristics concerning the nutrient budget are determined through soil organic matter, such as the cation exchange capacity, soil acidity, the capacity of binding organic chemicals (pesticides, herbicides, fertiliser, etc.), the release and sequestration of N, P, and S during decomposition of soil organic matter, and nutrient availability for soil micro-organisms (Volk and Loeppert, 1982). Besides the obvious impact of organic matter on

chemical soil properties which directly affect the quality of the soil for agricultural use (Kononova, 1961), organic matter also influences the physical characteristics of a soil with regard to accelerated soil erosion processes, as for example hydraulic conductivity (percolation and retention of soil water), soil structure (type and size of soil aggregates), and soil colour which influences albedo and soil temperature (Volk and Loeppert, 1982).

1.2.3. Detectable Soil Parameters

Soil parameters that affect the shape and nature of a soil spectrum are also referred as chromophores. They can be divided into chemical and physical chromophores (Ben-Dor et al., 1999). Chemical chromophores are those materials that absorb incident radiation in discrete energy levels. Usually the absorption process appears on a reflectance spectrum as a feature whose position is attributed to specific chemical groups in various structural configurations (overtone, combination modes, and electronic processes). All features in the VNIR-SWIR spectral regions have a clearly identifiable physical basis. In soils, three major chemical chromophores can be roughly categorized as follows: (1) minerals (mostly clay, iron oxide, primary minerals-feldspar, salt, and hard-to-dissolve substances such as carbonates, phosphates), (2) organic matter (fresh and decomposing), and (3) water (solid, liquid, and gas phases).

Physical chromophores are properties that affect the overall spectral region and a particular waveband position, or in other words, do not relate to the chemical functional group. Examples of these are particle size variation and refraction indexes of a material that changes from one illumination condition to another. A comprehensive review of each chemical and physical chromophore in soil is given in Irons et al. (1989, 1992), Ben-Dor et al., 1999, and Ben-Dor, 2002, as well as in Clark, 1999 and McBratney et al., 2006, elaborating on general minerals, some of which are found in the soil environment. In the following important chromophores are presented.

Iron and iron oxides

Iron is one of the most common minerals contained in soils (Hunt, 1980). In addition to several other nutrients (H, O, N, S, P, K, Mg and Ca), iron serves as an indicator for soil fertility, the usability of an area to cultivate specific crops and also an indicator for the duration and intensity of the pedogenesis, hence for the age of deposits (Torrent et al., 1980; Gardner and Pye, 1981; Blount et al., 1990). Iron is, in addition to H, O, N, S, P, K, Mg and Ca, an important soil nutrient. In soils, it is found in form of iron oxides that are concentrated in different soil layers (concretions), like rust spots or crusts in the profile.

One of the chemical tracers used for monitoring of soil genesis and formation is the free iron oxide (species and content) that may represent, for example, the soil rubification process. Rubification is defined as a stage in pedogenesis in which iron is released from primary minerals to form free iron oxides that coat quartz particles in soils with a thin reddish film (Buol et al., 1973). The free iron oxides coat the quartz particles and provide a reddish chroma to the matrix as well as stability (Ben-Dor and Singer, 1987). These iron oxides are,

together with aluminium oxides, important for the aggregate stability, since they serve as cementing agents between soil constituents (Ben-Dor et al., 2006).

Soil iron oxides are one of the main pigmenting agents of soil. Their continuous accumulation in the soil profile during pedogenesis produces intense soil colors. Yellowish-brown soil colors are caused by goethite, which is common in most soils. Hematite produces intense red soil colors and dominates soils of Mediterranean, subtropical and tropical regions (Cornell and Schwertmann, 1996). Small amounts of hematite can mask the yellow of goethite (Birkeland, 1999; Schwertmann, 1988; Torrent et al., 1983).

Quantification of iron oxides contained in soils using spectral measurements was also found to be possible as shown by several authors (e.g., Ben-Dor et al., 2006; Clark & Swayze, 1995; Palacios-Orueta et al., 1999; Torrent et al., 1983; Ben-Dor & Banin, 1990; Bartholomeus et al., 2006). Spectral determination of iron oxides is mostly based on the detection of the diagnostic absorption features of hematite (550, 630, and 860 nm) or goethite (480, 650, and 920 nm), which are the major iron oxide representatives in soils (Hunt et al., 1971; Morris et al., 1985).

The need for relatively high spectral resolution data to determine iron content using reflectance spectra has been discussed detailed in Ben-Dor et al. (1990).

The identification of secondary minerals such as Jarosite (iron sulfides) but also gypsum yield valuable information indicating the actual pyrite oxidation and associated acidification after remediation (Kemper & Sommer, 2003).

Correlation analyses revealed that the most spectral wavelength important for the successful prediction of heavy metals could be attributed also to the absorption features of iron and iron oxides (Kemper & Sommer, 2002).

Salinity

Soil salinity is one of the major factors affecting biomass production and is the principle cause of soil degradation (Csillag et al., 1993). Saline soils, typically shows high erosive characteristics with poor structure, low fertility, low microbial activity, and other attributes not conducive to plant growth (Ben-Dor, 1999). Salinization and soil degradation occur in areas where saline groundwater is elevated to where they approach the ground surface and evaporation exceeds precipitation. Either, induced by land clearing alone, referred to as dry land salinity, or by irrigation, referred to as irrigation induced salinity (Ben-Dor, 2008; Dehaan & Taylor, 2002).

Spectrally based studies by many researchers (e.g., Ben-Dor, 2002; Metternicht and Zinck, 1997, 2003; Taylor et al., 1994) have shown that detailed spectral information can directly and indirectly pinpoint saline-infected areas. For imaging spectroscopy Dehaan & Taylor (2002, 2003) demonstrated that mapping soil salinity from hyperspectral images is feasible via infrared absorption features and Taylor et al. (2001) could characterize dryland salinity by the occurrence of spectrally distinctive smectitic clays around surface salt scalds.

Halophytic vegetation is an indirect factor that facilitates detection of salt in soil using reflectance measurements.

Carbonate

Carbonates, especially calcite and dolomite, are mainly found in soils on lime-rich parent material or in a chemical environment that permits calcite and dolomite precipitation. In humid climates the carbonates are relocated from the upper soil layers or washed out into deeper horizons. In semi arid and arid climates carbonates can be found as crusts covering the soil surface or enriched in the upper soil layer.

Carbonates are important cation interchangers and influence directly the soil structure by coagulation, peptisation, and cementation of primary particles. These effects on the soil structure make them an important factor in the aggregate stability and soil erodibility. The detection of changes of carbonate content in the upper soil layer can be useful as an indicator of soil degradation processes.

The C-O bond, part of the CO_3 -radical in carbonate, is the spectrally active chromophore (Ben-Dor, 1990). The major overtones and combination modes in the SWIR region were summarized by Vander Meer (1995) and Gaffey (1986), pointing out significant spectral differences between calcite and dolomite. Kruse et al. (1990) and Ben-Dor & Kruse (1995) used this distinction to map between calcite and dolomite using airborne spectrometer data.

Clay Minerals

The composition of the clay fraction and clay minerals in the soil are influenced by many different factors. They depend on parent material, climate, soil pH-value, composition and concentration of the soil solution, degree of soil development, and the soils age. Soils covering parent material containing clay minerals are dominated by illite and smectite (e.g., montmorillonite). Over parent material not containing clay minerals (e.g., magmatites) the clay minerals in the soil are always of pedogenic nature. Their composition is determined by the mineral component of the parent material and the weathering rate of the soils. Soils with a higher proportion of the clay fraction have favourable chemical characteristics but unfavourable physical characteristics. Clay minerals are, as well as humic substances, important cation interchangers. They affect nutrient supply of plants and soil characteristics like soil structure, water supply, distribution of porosities, biological activity, and, thus, directly the erodibility of soils.

Of all clay minerals only the hydroxide group is spectrally active in the VNIR-SWIR region (Hunt, 1979). The OH group can be found either as a part of the mineral structure (lattice or bound water) or as part of a thin water molecule attached to the mineral surface (adsorbed water) (Ben-Dor, 1990).

Three major spectral regions are active for clay mineral in general (features located at 1400, 1900, and 2200 nm). The strong absorption bands at 1400 and 1900 nm are due to bound water, typical of montmorillonite, while strong OH bands at 1400 and 2200 nm are typical of kaolinite (Hunt and Salisbury, 1970). The presence of a 1900 nm band is also key to the swelling potential as it indicates molecular water in the sample (2:1 layer clay, montmorillonite, or illite), whereas its absence but the presence of a 1400 nm band indicates that only OH is present (kaolinite, 1:1 layer clay) (Kariuki, 1999; Chabrilat *et al.*, 2001). Chabrilat & Goetz (2006) and Chabrilat et al. (2002) also demonstrated that expansive clay mapping is feasible from hyperspectral images.

Taylor, 2004 described how the shape of the hydroxyl absorption feature at 2200 nm (depth and width) changes with increased soil salinity forming the basis for the development of methodologies for saline soil mapping. This occurs both laterally, around saline discharge zones, and vertically, in soil profiles where salt has accumulated at the surface as a result of evaporation. An asymmetry to shorter wave-lengths, due to kaolinitic minerals, is replaced by an asymmetry to longer wavelengths, characteristic of smectites. This corresponds to the observed increased frequency of swelling clays around saline discharges, which often leads to dispersive soils and subsequent soil erosion.

Organic Carbon

Soil organic matter has a great influence on the physical (soil structure and porosity), chemical (complexing agent, sorbent), and biological (source of nutrients to plant and microorganisms) properties of soil. Soil organic carbon also plays an important role of the C cycle (Schlesinger, 1990). The measurement of organic carbon content in the soil is an important indicator to ascertain the soil organic matter content. The C/N (carbon/nitrogen) ratio serves as a measure for the micro-organic decomposition of the organic material in the soil. Soil organic matter is a mixture of dead materials from plants, animals, and secretion substances of organisms at different stages of decomposition. The sequence of organic matter decomposition in soils is strongly determined by micro-organism activity in the upper soil horizons. The mostly positive electric charge of the macro-molecules of the humic substances supports the aggregation of clay particles and thereby the formation of clay-humus-complexes. Clay-humus-complexes are important for the aggregate stability and erodibility of the soil. It is possible to draw conclusions from detected increase or decrease of organic matter in the upper soil layer on changes in aggregate stability and soil erodibility. Typical bare soils in land use areas not masked by dense vegetation contain about 1-6% organic matter, 50% of which are organic carbon (Scheffer und Schachtschabel, 1992).

General models related to organic matter dynamics indicate that the physical characteristics of a soil reflect the balance between regenerative or degenerative processes of soil structure development. Stable macro-aggregates (> 250 µm) formed by inorganic compounds are, in general, held together by iron and aluminium oxides and occur predominantly in oxisols (Oades and Waters, 1991). Otherwise, stable macro-aggregates are formed by soil organic matter such as fungal hyphae, fibrous roots, and polysaccharides. They rather occur under pasture or where organic residues have been added to the soil (Lynch and Bragg, 1985). The stability of macro-aggregates increases with the amount of stable micro-aggregates (Tisdall and Oades, 1982; Tisdall, 1996). Since soil erodibility (i.e., the resistance to mechanical detachment and breakdown of soil aggregates, and the ability to accept rainfall as infiltration) is greatly influenced by the structural organisation of the soil, it is obvious that highly calcareous silty Mediterranean soils become, in the absence of clay, highly dependent on organic matter (Imeson, 1995). Increased organic matter concentrations render these soils more favourable because of better aggregation, higher infiltration and water-retention, and increased nutrient availability. Also, better infiltration of rainfall and the formation of macro-aggregates are among the most important soil properties to increase their resistance to accelerated erosion.

Particularly in the case of low clay contents in soils the production of stabilising agents is primarily driven by causal loops involving organic matter production through biological activities (Dalal and Bridge, 1996). Since the agents of stabilisation are consumed or degraded in the soil they need to be periodically replenished by biological activity. If the balance between the amount of organic carbon being produced by plants is positive in relation to that being consumed by micro-flora, then the soil will produce either more or larger agglomerations of particles, thereby generating the positive feedbacks of increased aggregate stability, water and nutrient availability required for sustained plant growth and reduced erodibility (Imeson et al., 1996).

Because of its extreme biochemical heterogeneity, soil organic matter is often separated into operationally defined fractions related to specific biogeochemical processes of interest (Herbert and Bertsch, 1995).

Organic matter absorbs the infrared (IR) light across wide parts in the near- and mid-IR regions due to heterogeneity of the structure with several functional groups. The strong absorption of IR light by soil minerals in the same regions can interfere in the IR-spectra of soil organic matter. Therefore, soil organic matter is often characterized by minor peaks or by subtle changes to the infrared spectra of soil, such as peak broadening, frequency shifts, and intensity changes. The complexity of IR spectra of soil organic matter and highly overlapping bands with other mineral components in soil overburden the simple univariate calibration with a single selected peak. However, with development of chemometrics and spectroscopic techniques it is possible to construct a reliable calibration model to predict chemical and physical properties in soil.

Biological Soil Crusts

In many dryland ecosystems biological crusts are dominating the soil surface (Hill et al., 1998). The ecological importance of these crusts is related to their resistance against erosion caused by wind or surface runoff, and the protection of infiltrated rain water against excessive evaporation. Hyperspectral sensor systems provide a good potential to assess the existence of biological crusts and to differentiate various types of crusts, thereby providing important information on areas of stability and disturbance in arid ecosystems.

Soil Colour

Soil colour is still one of the indispensable characteristics for classification or composition study (Boul et al., 1973), especially when soil is studied with remote sensing techniques. Soil colour describing visible chromophores is influenced by moisture, roughness, organic matter (black, brown-black, grey colours) content, minerals like Fe/Mn-oxides (brown, red, brown-black colours), silicates, carbonates, phosphates, and sulphides. These relations are helpful to predicate the mineralogical content, salt content, electric conductivity and other characteristics of the considered soil material. It is possible to identify soil erosion by detecting changes in soil colour at the surface.

Because it represents the integrated reflectance spectral information between approximately 400 and 700 nm (VIS region), it averages all chromophores across this region and therefore

cannot constitute the most comprehensive information for analyzing the soil's properties. In addition, it does not cover other parts of the electromagnetic radiation (EM) that are associated with important soil chromophores (e.g., NIR-SWIR-TIR). Nevertheless, soil color does provide a qualitative impression of properties such as organic matter, water status, the content of iron oxides

Soil Moisture

Soil water content is an important component that influences macro- and meso-scale processes. The agricultural capacity of an area is directly affected by soil moisture, especially in arid regions. In temperate and humid regions soil water content is important in determining flood risks and pollutant transport through the soil. The albedo represents the intrinsic optical properties of soil materials. As soils are drying an increase of albedo is noticeable. There are relationships between soil moisture, erosion resistance, and evaporation into the atmosphere. Other functions describe relations between canopy resistance and soil moisture. Also, for bare soils it is customary to express the resistance to evaporation as a function of soil moisture. Estimations of evaporation and evaporation resistance provide possibilities to describe the natural variability of the evaporation process (Bastiaansen et al., 1997) that is important for estimating regional energy and water balances.

Haubrock et al., 2004, 2008 have developed and successfully tested a new model for determining soil moisture by means of remote sensing techniques. It was based on a combination of multitemporal high-spatial resolution image spectroscopy observations with field and laboratory spectral studies, along with hydrological measurements. The method is termed the Normalized Soil Moisture Index, and it was tested for the best spectral prediction of soil moisture content in the field using the 400 to 2450 nm spectral region. The coefficient of determination R^2 is 0.61 (up to 0.71) for natural field samples, taking into account the influence of different environmental factors: heterogeneous soil types and related field moisture content, variable soil water profiles, and the presence of soil crust and vegetation cover. This index allows the production of surface soil moisture maps, generated from HyMap airborne images

Another novel approach for reconstructing the soil spectral signature was through the use of various water film depths related to moisture content. Bach & Mauser (1994) were able to simulate the reflectance change of the soil spectra from dry to moist. They combined the model by Lekner & Dorf, 1988 for internal reflectance with the absorption coefficients from Palmer & Williams, 1974 into Lambert's law (or Beer's Law) to simulate the moist reflectance R from the dry reflectance R_0 by the exponential of the absorption coefficient and an empirically determined "active thickness". They applied this process for predicting the water contents within an AVIRIS image of a partially irrigated field and a dark organic soil field in the Freiburg test site in Germany from the image pixel spectra of dry and moist soils. The active thickness and water absorption coefficients predicted the amount of the soil's water content to a high R^2 of 0.88.

Soil roughness

Soil surface roughness is a crucial measurement in the assessment of soil erosion processes. It is the most important factor influencing the directional reflectance of a bare soil (Jaquemoud et al., 1992). Particle-size differences influence on the shape of spectra has been shown in various studies (Baumgardner et al., 1985; Gaffey, 1986; Hunt and Salisbury, 1970; van der Meer, 1995). Generally reflectance increases and the contrast of absorption feature decreases as particle or aggregate size decreases (Bowers & Hank, 1965; Hunt, 1980; Stoner & Baumgardner 1980). The inverse relationship between particle size and soil reflectance is a characteristic of transparent materials and most silicate minerals behave transparently in the SWIR region (Salisbury & Hunt, 1968). The common experience that clayey soils often appear darker to the eye than sandy soils may be explained in the part by the different mineralogies of clay and sand particles, but may also be due to the tendency of clay particles to aggregate (Atzberger, 2002).

The reflectance of a bare soil is highly correlated with shadows created by soil surface particles and depends on the roughness and measurement conditions. These findings seems logic if one considers that the surface becomes smoother when particle size decreases. Contrary, coarse aggregates, having an irregular shape, form a complex surface with large number of interaggregate spaces. When light falls on large, irregularly shaped aggregates, most of the incident flux penetrates into light traps and is completely absorbed within there (Baumgardner et al., 1985). The understanding of light diffusion between soil particles should help to gain information on roughness.

1.2.4. Parameter Retrieval Strategies

A major difference to geological applications is that soil constituents can be assessed rather from the spectral continuum than based on specific absorption features. Most parent materials differ spectrally from developed soil substrates, mainly due to the absence of specific spectral absorptions and increased albedo levels. Truncated profiles may be characterised by decreasing or increasing amounts of soil components.

Bi-directional soil reflectance in the wavelength range between 0.4 and 2.4 μm is a cumulative property, derived from the inherent spectral behaviour of the heterogeneous combination of minerals, water and organic matter. Using statistical regression methods several authors established relationships between soil reflectance and organic matter (Krishnan et al., 1980, Dalal & Henry, 1986), hygroscopic moisture (Dalal & Henry, 1986), clay content, specific surface and carbonate content (Ben-Dor & Banin, 1990, 1994). Some of the most common used techniques enabling the retrieval of the important hidden information in soil spectra are presented in the following.

Statistical Regression Analysis

There exist several different techniques that are very popular by soil scientists.

Linear Regression is a form of regression analysis in which the relationship between one or more independent variables and another variable, called dependent variable, is modeled by

a least squares function, called linear regression equation. This function is a linear combination of one or more model parameters, called regression coefficients. A linear regression equation with one independent variable represents a straight line. The results are subject to statistical analysis.

Multiple Linear Regression (MLR) attempts to model the relationship between two or more explanatory variables and a response variable by fitting a linear equation to observed data.

Stepwise Multiple Linear Regression (SMR) has proved to be an extremely useful computational technique in data analysis problems. This procedure has been implemented in numerous computer programs and overcomes the acute problem that often exists with the classical computational methods of multiple linear regression. This problem manifests itself through the excessive computation time involved in obtaining solutions to the $(2^N - 1)$ sets of normal equations that arise when seeking an optimum linear combination of variables from the subsets of the N variables. The procedure takes advantage of recurrence relations existing between covariances of residuals, regression coefficients, and inverse elements of partitions of the covariance matrix. The application of these recurrence formulas is equivalent to the introduction or deletion of a variable into a linear approximating function which is being sought as the solution to a data analysis problem.

Partial Least Square Regression (PLR) is a recent technique that generalizes and combines features from principal component analysis and multiple regression. It is particularly useful when we need to predict a set of dependent variables from a (very) large set of independent variables (i.e., predictors).

Artificial Neural Networks (ANNs)

These networks represent parallel computational models comprised of densely interconnected adaptive processing units. A very important feature of these networks is their adaptive nature, where "learning by example" replaces "programming" in solving problems. This feature makes such computational models very appealing in application domains where the analyst has little or incomplete understanding of the problem to be solved, but where training data are readily available. For classification purposes, feed-forward network types such as **Multilayer-Perceptron (MLP)** or **Radial-Basis-Function Networks (RBF)** are used. Both allow an universal function approximation since they represent highly complex, non-linear regression models (Hartman et al., 1990); (Hornik, 1991). The parameters of these models are estimated by linear and non-linear optimisation techniques based on training samples. Due to the high flexibility of these models, user experience is required for network design and parameter estimation.

Support Vector Machines (SVM) can be an alternative to ANNs, as they possess similar characteristics. However, in spite of being very flexible and accurate they all have the drawback, that the extracted decision rules are not forthcoming due to the black box character of these techniques. The MLP and a SVM-tool is available within the ENVI-Software.

Spectral Mixture Analysis (SMA)

This technique, also referred to as **Linear Spectral Unmixing (LSU)**, is based on the assumption that most of the spectral variation in hyperspectral images is caused by linear/non-linear mixtures of a limited number of surface materials. The approach models the hyperspectral surface reflectances as a mixture of representative prototype spectra, the so-called spectral endmembers (e.g., soil, minerals, vegetation, water, and shade as an illumination component). The mixing can result from a collection of relatively large (yet still sub-pixel) areas of pure species, or from collections of many, very small (even microscopic) regions of these species. In the latter case the radiometric mixing can occur as a volume effect and as such would be non-linear.

In recent years, many authors have proposed and used a more complex model where both the number and the set of EMs vary dynamically on a per-pixel basis (Roberts et al. 1998), which has become known as **Multiple Endmember Spectral Mixture Analysis (MESMA)**. The idea consists in restricting the large set of possible EMs to a small set of appropriate EMs which can be different for each pixel, thereby allowing an accurate decomposition using a virtually unlimited number of EMs. These spectra are chosen to represent the spectral variability of a larger area of interest but would over determine the spectral signal of most of the single pixels.

An improved strategy called **Variable MESMA (VMESMA)** increase the flexibility and accuracy of MESMA (Garcia-Haro et al., 2005) considering a zonal partition of the area and a zone-dependent choice of different EM submodels and methods. This method allows for the definition of standard and repeatable pathways to incorporate information dynamically derived from the unmixing results with other sources of data in order to optimize the algorithms and to increase the flexibility of the modeling approach. VMESMA is conceived as an iterative or feedback process, in which unmixing performance may be potentially improved in each stage until an optimum level is reached. The LSU approach is implemented in the ENVI software.

Partial Least Square Regression (PLSR)

Multivariate regression methods like partial least squares regression (PLSR) enjoy large popularity, especially in spectroscopy, because they have been designed to confront the situation that there are many, possibly correlated, predictor variables (in this case many wavelength), and relatively few samples. In fact, the origin of PLSR lies in chemistry (e.g. Wold, 2001; Martens, 2001). The field of near-infrared (NIR) spectroscopy, with its highly overlapping lines and difficult to interpret overtones, would not have existed but for a method to obtain quantitative information from the spectra.

In soil spectroscopy PLSR is used to split spectral data (X) and soil property data (Y) into a new smaller set of latent variables and their scores that best describe all the variance in the data. Therefore PLS decomposes X into orthogonal scores T and loadings P and regress Y not on X itself but on the scores T. Different to principal component regression (PCR), where for the scores only information on X are taken into account (and therefore may be suboptimal for prediction purposes), PLSR aims to incorporate information on both X and Y in the definition of the scores and loadings. Though, these scores and loadings are chosen in such

a way to describe as much as possible of the covariance between X and Y, where PCR concentrates on the variance of X (Mevik & Wehrens, 2007).

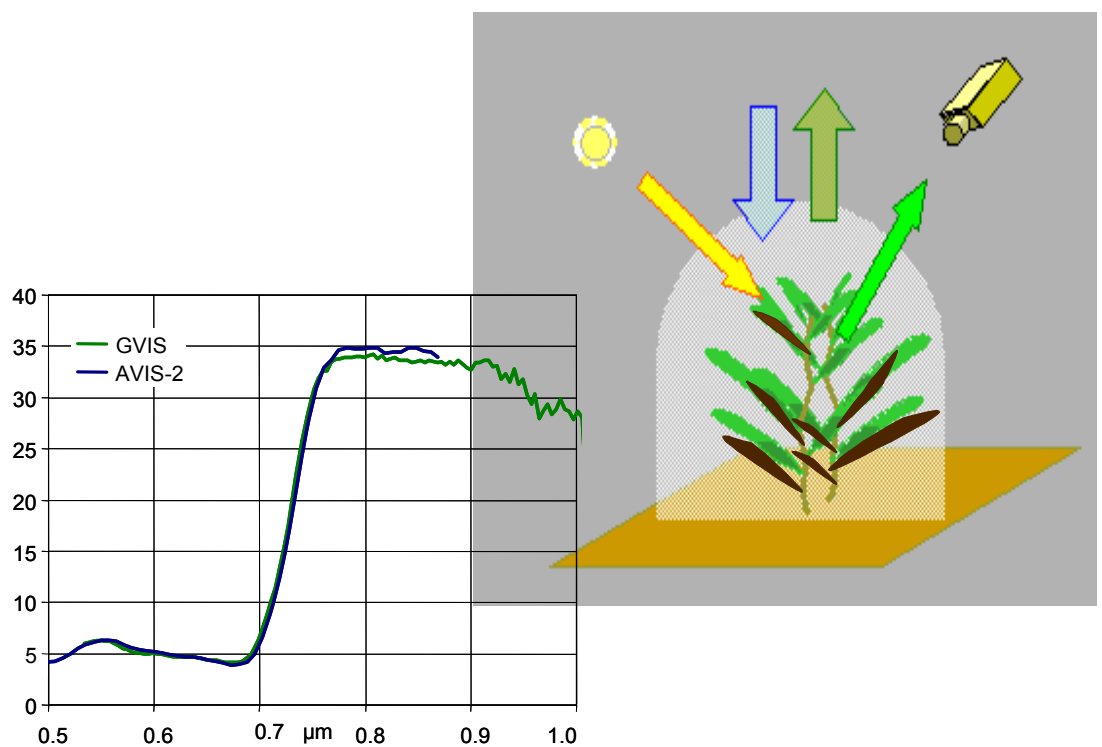
1.2.5. Priorities and Recommendation for Implementation

In contrast to geological applications, the analysis of soils demands a complete different approach. Minerals showing diagnostic absorption features can be automatically identified. Such an automated process is not feasible for soil applications as the spectral characteristics are highly variable and many parameters can only be retrieved using an indirect approach. The extraction of such hidden information from spectra requires detailed knowledge about field samples and their chemical composition. Hence, statistical regression analysis is the most popular retrieval approach in soil science. Such algorithms should be provided to the EnMAP users in the toolbox as they do not exist so far in commercial image processing software (e.g. ENVI). The quality of the input of such regression models is decisive for a good result. Hence, new methods for automated feature extraction are necessary in the same manner. Their combination with the parameter modeling will help the user to find the optimum result.

Improved algorithms for classification or spectral mixture analysis are explicitly not indispensable for soil studies, but should be discussed and selected considering the demands from other research fields (e.g. geology, forest, and land use).

2. Review of Algorithms and Products with Relevance for the EnMAP Toolbox Issue – Agriculture

Heike Bach, Annette Wagner



List of Acronyms

ACORN	Atmospheric Correction Now
ANN	Artificial Neural Networks
CAI	Chlorophyll Absorption Integral
CAI	Cellulose Absorption Index
CCI	Canopy Chlorophyll Content Index
CF	Chlorophyll Fluorescence
CWC	Canopy Water Content
DM	Dry Matter
EO	Earth Observation
EWT	Leaf Equivalent Water Thickness
FLD	Fraunhofer Line Depth
FLEX	Fluorescence Explorer
FRI	Fluorescence Ratio Indices
IRI	Infrared Index
LAI	Leaf Area Index
LUT	Look-up Table
MPLS	Modified Partial Least Squares Regression
MLR	Multiple Linear Regression
MR	Multiple Regression
MCARI	Modified Chlorophyll Absorption Ratio Index
MSRpi	Modified Spectral Ratio Planar Index
MTVI	Modified Triangular Vegetation Index
N	Nitrogen
NDLI	Normalized Difference Lignin Index
NDVI	Normalized Difference Vegetation Index
NIR	Near Infrared
NNT	Neural Networks
NPQ	Non-photochemical Quenching
PLS	Partial Least Squares Regression
PQ	Photochemical Quenching
PRI	Photochemical Reflectance Index
QNT	Quasi-Newton Algorithm
RAMI	The Radiative Transfer Model Intercomparison exercise
REIP	Red Edge Inflection Point
RT	Radiative Transfer
SAIL	Scattering by Arbitrarily Inclined Leaves
SIPI	Structure Insensitive Pigment Index
SLC	Soil Leaf Canopy
SR	Simple Ratio
SVR	Support Vector Machines Regression
SWIR	Shortwave Infrared
TCARI	Transformed Chlorophyll Absorption in Reflectance Index
VI	Vegetation Index
VIS	Visible

2.1. Introduction

A literature review of research in hyperspectral data analyses in the field of agriculture is provided in this report. Hyperspectral algorithms are investigated and their applicability and relevance for the future ENMAP instrument is assessed. This review is based on a selection of approx. 140 relevant papers published during the last 10 years in high ranking journals of remote sensing and agriculture. The main criteria for the review were:

The algorithms should make special use of hyperspectral measurements, since these will be delivered by ENMAP.

The methods should have been applied in an agricultural application.

The algorithms and methods should be as far as possible geographically and temporally transferable.

The methods should allow a high degree of automation.

If an algorithm provides a retrieval result (e.g. chlorophyll content), a validation is required with a good level of accuracy.

The methods should deliver land surface parameters that are of practical relevance for agricultural applications.

As conclusion advices for algorithms and methods to be implemented in the planned ENMAP toolbox are provided.

2.2. Overview of Findings

Since the methods should have practical relevance, they need to address crop parameters of interest for agriculture. These crop parameters were differentiated in 9 classes as illustrated in Figure 1. This graph illustrates the relative frequency of the investigation of the respective parameter, highlighting that the Leaf Area Index (LAI), chlorophyll and nitrogen content as well as crop stress were studied in most cases and are of central interest.

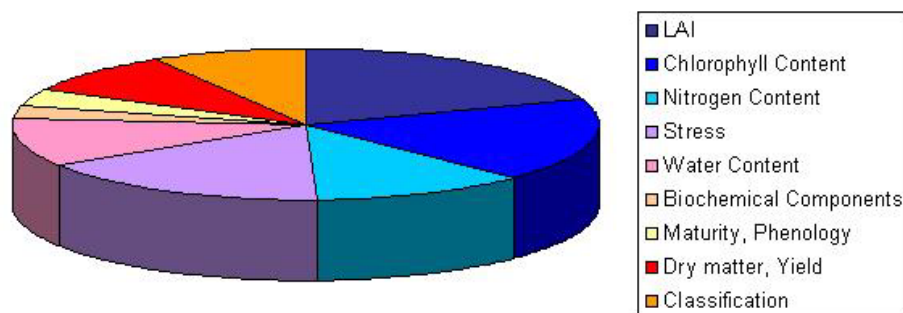


Figure 1: Distribution of agricultural parameters investigated in the reviewed agricultural hyperspectral studies

Hyperspectral airborne or spaceborne data is still only rarely available to scientists. This explains why almost 50% of the agricultural studies use data from field spectrometers (see Figure 2). Most others are based on airborne acquisitions of a range of sensors. Satellite sensors (CHRIS and Hyperion) can only contribute slightly due to their restricted availability and also limited data quality. It can thus be expected that the availability of a sophisticated spaceborne hyperspectral sensor, like ENMAP, will push forward remote sensing

applications in agriculture and will contribute to an improvement of operational applications in agriculture.

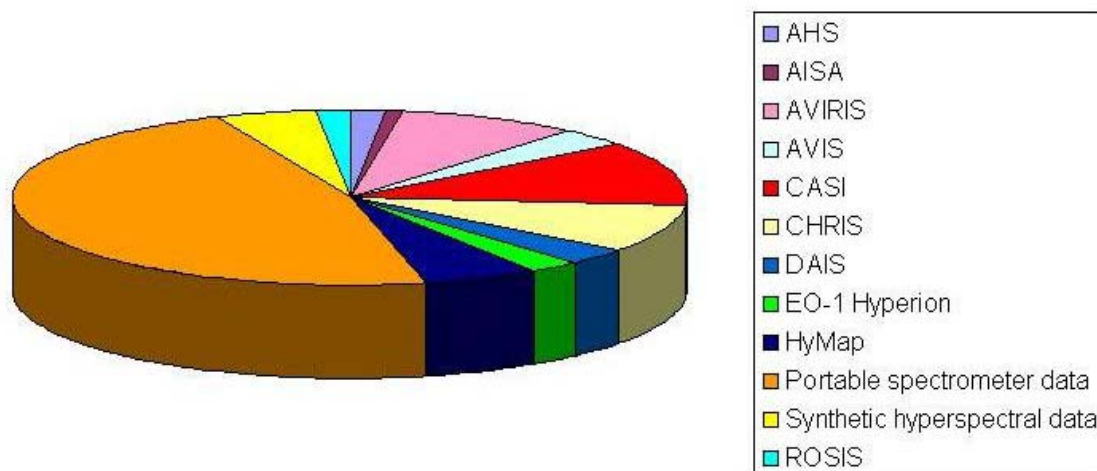


Figure 2: Distribution of applied sensors in the reviewed agricultural hyperspectral studies

2.2.1. Overview of Techniques

Common approaches to estimate vegetation parameters from hyperspectral remotely sensed data can be classified into **explicit** and **implicit** methods.

Implicit methods such as empirical or statistical approaches attempt to obtain a relationship between a vegetation parameter of interest (e.g. LAI measured in situ) and the leaf or canopy reflectance, or some form of vegetation index (VI). The accuracy of the measurements and the range of conditions that were taken into account for the establishment of a relationship determine to a large extent the validity and transferability of the relationship (Sims and Gamon 2002). Traditional techniques of linking spectral information to the variable of interest are **Simple Regression** (SR) or **Multiple Regression** (MR) techniques. More recent approaches include **Artificial Neural Networks** (ANNs), **Partial Least Squares Regression** (PLS) and Modified **Partial Least Squares Regression** (MPLS).

The simplicity and computational efficiency of **empirical** or **statistical approaches** would make them desirable especially for large-scale remote sensing applications, granted that the statistical or empirical relationship remains valid. A fundamental problem however, is their lack of generality, as they are mostly restricted to the prevailing conditions of the conducted study. For direct large-scale operational use and the application to different conditions or in different phenological seasons they are recognized as being inadequate (Houborg et al. 2007, Meroni et al. 2004). In a recent study concerning the angular sensitivity of VIs from CHRIS/Proba data, Verrelst et al. (2008) concluded that nearly all tested indices (e.g. NDVI, SIPI, PRI) manifested a prominent reflectance anisotropy and pointed out the need for a standardization of vegetation indices in order to establish confidence in the reliability of their use. Besides the sun and view geometry, also soil reflectance has an impact on the canopy reflectance and needs to be considered for derivation of crop parameters. Possible solutions to overcome these problems using implicit methods are the continuum removal and the use of derivatives. These do not use the absolute values of reflectance but their relative shape.

Explicit methods are **physically based approaches** involving the use of **radiative transfer or canopy reflectance models**. Using physical laws, they attempt to provide an accurate description of the transfer and interaction of radiation at the soil surface, inside the leaves and the canopy. The complexity of these models ranges from simple non-linear to complex radiative transfer models in realistic three-dimensional vegetation canopies (Kimes et al. 1998). A lot of studies at leaf scale use the model PROSPECT (Jacquemoud et al. 2000) or LEAFMOD (Ganapol et al. 1998) in this context. For simulations on canopy scale, leaf scale models are often coupled with canopy scale radiative transfer models, like KUUSK (Kuusk, 1998). Most studies operate with the SAIL (Scattering by Arbitrarily Inclined Leaves) model developed by Verhoef (1984) or modified versions of the SAIL model such as SAILH (hot spot extension to SAIL) (Verhoef, 1985) or SLC (Verhoef and Bach 2007). SLC stands for “**Soil Leaf Canopy**” and is a recent extension of SAILH to account for heterogeneous canopies allowing the simulation of two spatial layers with different optical properties. Incomplete vegetation coverage can be considered applying a non-linear mixing of background and vegetation cover. Additionally, a flexible soil background model is integrated in SLC that also considers soil BRDF and moisture effects.

Figure 3 shows a schematic representation of canopy reflectance simulations that use PROSPECT and SAIL in a model chain. More than 90% of all studied publications that use radiative transfer models apply such a combination of PROSPECT with a SAIL derivative.

Radiative transfer models are applicable in both forward and inverse modes. In forward mode, they are often used for the generation of large databases of reflectance spectra with wide ranges and combinations of input variables that describe the biochemical and biophysical plant properties (Blackburn 2007). A comparison of four radiative transfer models in direct and inverse modes, where the leaf optical properties model PROSPECT is combined with the canopy reflectance models SAIL, IAPI, KUUSK, and NADI (New Advanced Discrete Model) is presented by Jacquemoud et al. (2000). The results in forward and inverse mode showed no distinct difference. All model combinations were found to provide similar results.

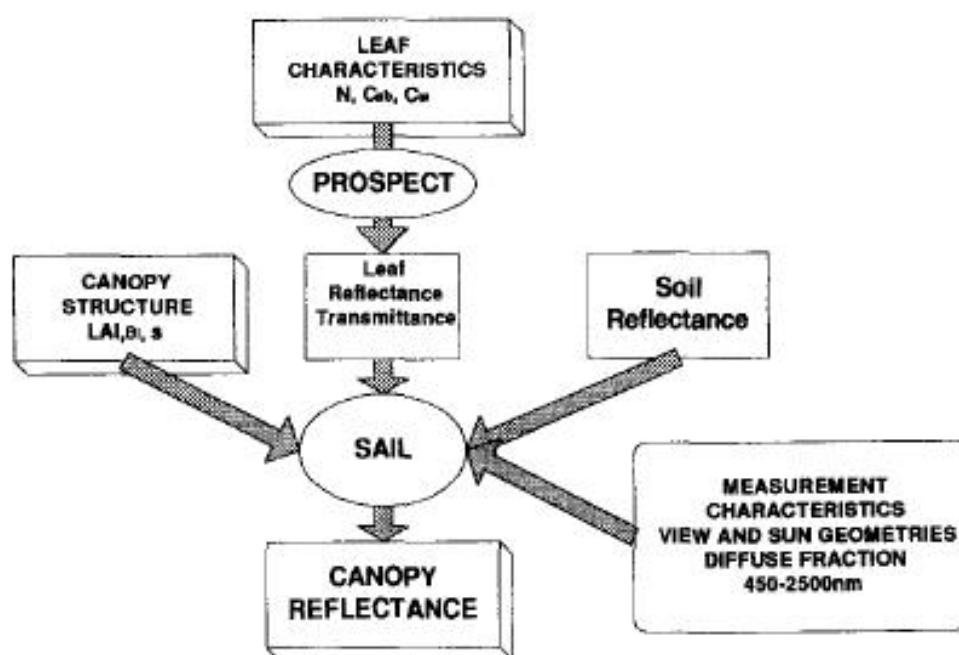


Figure 3: Schematic representation of the PROSPECT+SAIL canopy reflectance model (Jacquemoud et al. 1995)

The observation that most of the presently available canopy reflectance models deliver very comparable results when using the same input variables was also confirmed within the RAMI experiment. The Radiative Transfer Model Intercomparison exercise (RAMI) has been committed to a systematic voluntary evaluation of canopy reflectance models since 1999. Up-to-date results are published regularly (Pinty et al. 2001, Widlowski et al. 2007).

In order to use physically based models for the retrieval of vegetation characteristics from observed reflectance data, they have to be inverted. For model inversion different techniques have been proposed. The most dominant are **numerical optimization methods**, **look-up table** (LUT) approaches, **artificial neural networks** and recently **support vector machines regression**. The right inversion technique and the type and quality of remotely sensed data are the most crucial factors for the accuracy of physically based models for the retrieval of vegetation characteristics from reflectance data. A comparison between the three inversion methods can be found in Combal et al. (2002). A drawback of the numerical optimization approach is that it cannot guarantee a stable and optimum inversion, as the search algorithm may get trapped in local minima before reaching the global minimum. Additionally, the technique is computationally intensive, in particular when using complex radiative transfer models. The retrieval of biophysical variables for large geographic areas with this inversion technique is therefore considered as being unfeasible. LUT and neural network approaches are less computationally intensive. However, for proper training (artificial neural networks) and representation (LUT), a large database of simulated canopy reflectance spectra is needed in order to achieve a high degree of accuracy. Neural network inversion seems to be less affected by model uncertainties (Combal et al. 2002), but are considered to be more difficult in the adaptation to changing local conditions (Dorigo et al. 2007).

2.2.2. Statistical Versus Physical Approach

Concerning the exploitation of hyperspectral characteristics, parameter retrieval based on Partial Least Squares regression models, artificial neural networks or radiative transfer models use nearly the complete spectral information of a sensor, whereas most vegetation indices are mainly based on only few spectral wavebands. As radiative transfer models are physical models, they can be applied to variable conditions and times. Statistical approaches are not automatically valid for variable conditions. An advantage of statistical approaches is their simplicity and computational efficiency. Radiative transfer models, on the contrary, are complex models, and especially the model inversion process faces some problems: (i) the fact that there generally is no analytical solution of the inverse problem which makes the inversion with numerical optimization techniques very time consuming, (ii) the ill-posed nature of the inversion process, leading to unstable inversion results because some model parameters (e.g. LAI and average leaf inclination angle) counterbalance each other (Atzberger et al. 2003, Combal et al. 2002). Solutions for the first problem can be found in a restriction of the inverse problem or in using either artificial neural nets (ANNs) or look-up-tables (LUT), which implies that the radiative transfer model is only used in the forward mode to build a synthetic data set which is then used to train the artificial neural net or build a look-up table. Concerning the ill-posed nature, solutions include the use of prior information (Bach et al. 2000, Combal et al. 2002) or the derivation of additional information from the remote

sensing data itself, such as spectral properties from surrounding pixels (Atzberger et al. 2003, Darvishzadeh et al. 2008).

Sample simulation results using the canopy reflectance model SLC are illustrated in Figure 4. The effect of changes of LAI, crown cover, leaf slope, changes in chlorophyll and water content of leaves as well as of soil moisture is illustrated. The illustrated spectral range corresponds with the specifications of ENMAP.

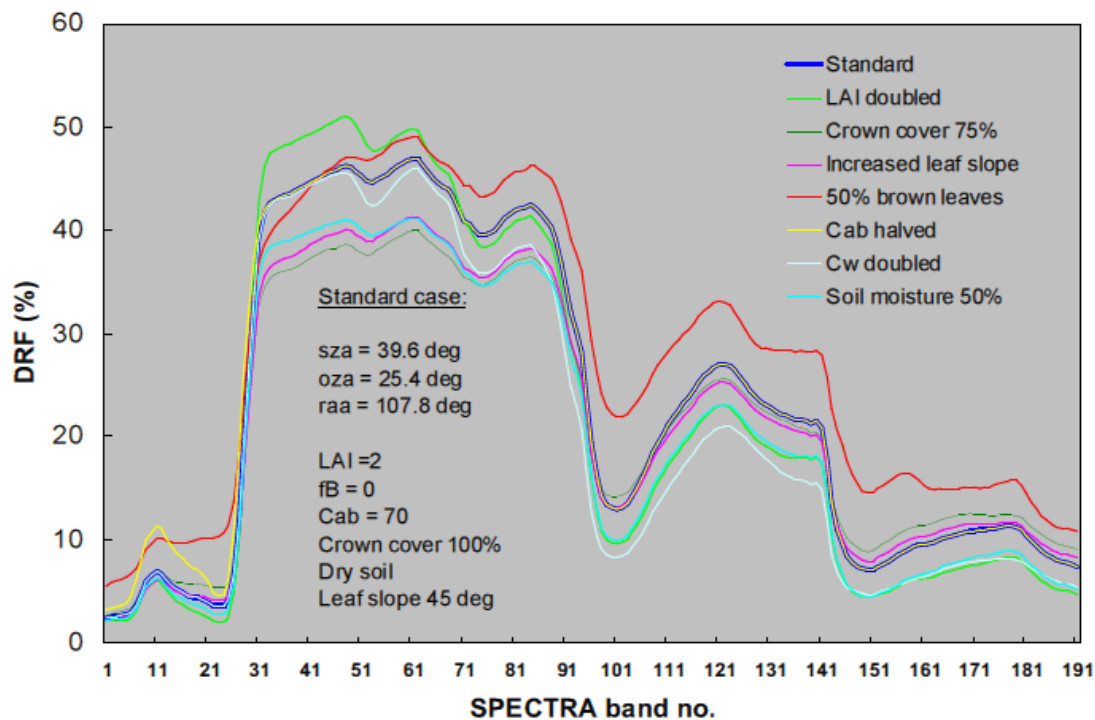


Figure 4: Various causes and their spectral effects on near-nadir hyperspectral acquisitions simulated with SLC (Verhoef, 2003)

Figure 5 illustrates the occurrence of statistical approaches in comparison to modelling approaches in the current literature review. Obviously the simple statistical approaches still dominate in agricultural research. Both approaches have benefits and limitations so that a recommendation for the choice of either of them depends on the specific situation for which its application is desired. It can however be concluded that transferable, generally applicable or automated procedures for agricultural information retrieval from hyperspectral data will require the application of radiative transfer models. The state of art in the forward mode of these models is already well developed. As Figure 5 shows, these models are nevertheless only rarely used. This might be caused by their complex nature. Easy to use and user friendly model tools might be a solution to overcome this acceptance problem. Additionally, in order to find the best way for the inversion of the radiative transfer models, further research and development activities are still required.

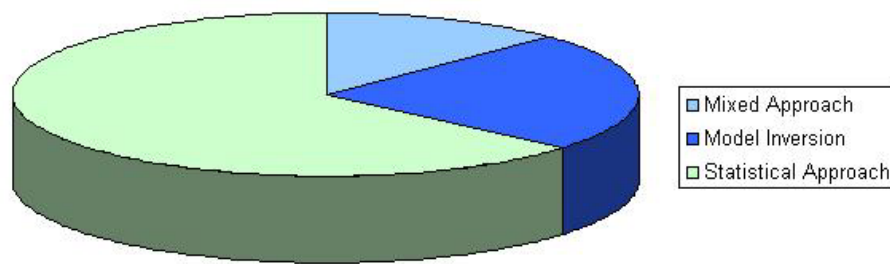


Figure 5: Application of statistical approaches versus modelling approaches in the current literature review.

2.2.3. Overview of Approaches Using Hyperspectral Indices

Statistical approaches, which as shown above are still mostly used, correlate spectral indices retrieved from hyperspectral data with field measurements of crop characteristics. The list of applied indices is very large. A summary of the most important indices (more than 30), their calculation rules, the authors who applied them, as well as the crop parameter it was correlated to is compiled in this review. The concluding list is provided in Appendix 1 (Chapter 12).

For visualization of these hyperspectral indices the spectral bands that are used for their calculation were compiled and illustrated in Figure 6. The different symbols refer to the crop parameter the index is correlated to. For LAI retrieval, indices use bands in nearly the whole visible region ($> 500\text{nm}$), NIR and even SWIR region (1250 nm), since the development of leaves has strong impact on the reflectance of the whole spectral range. For the derivation of chlorophyll content wavelengths at $530\text{-}630\text{ nm}$ and $700\text{-}750\text{ nm}$ in the red edge region (corresponding to the lower and upper flanks of chlorophyll absorption) are used since they are most sensitive to normal-range chlorophyll concentrations. For low concentrations of chlorophyll also wavelengths corresponding to the centre of the major absorption features i.e. $660\text{-}680\text{nm}$ are valuable. For the estimation of nitrogen content the spectral ranges are very similar to the ones of chlorophyll, since both crop parameters are correlated.

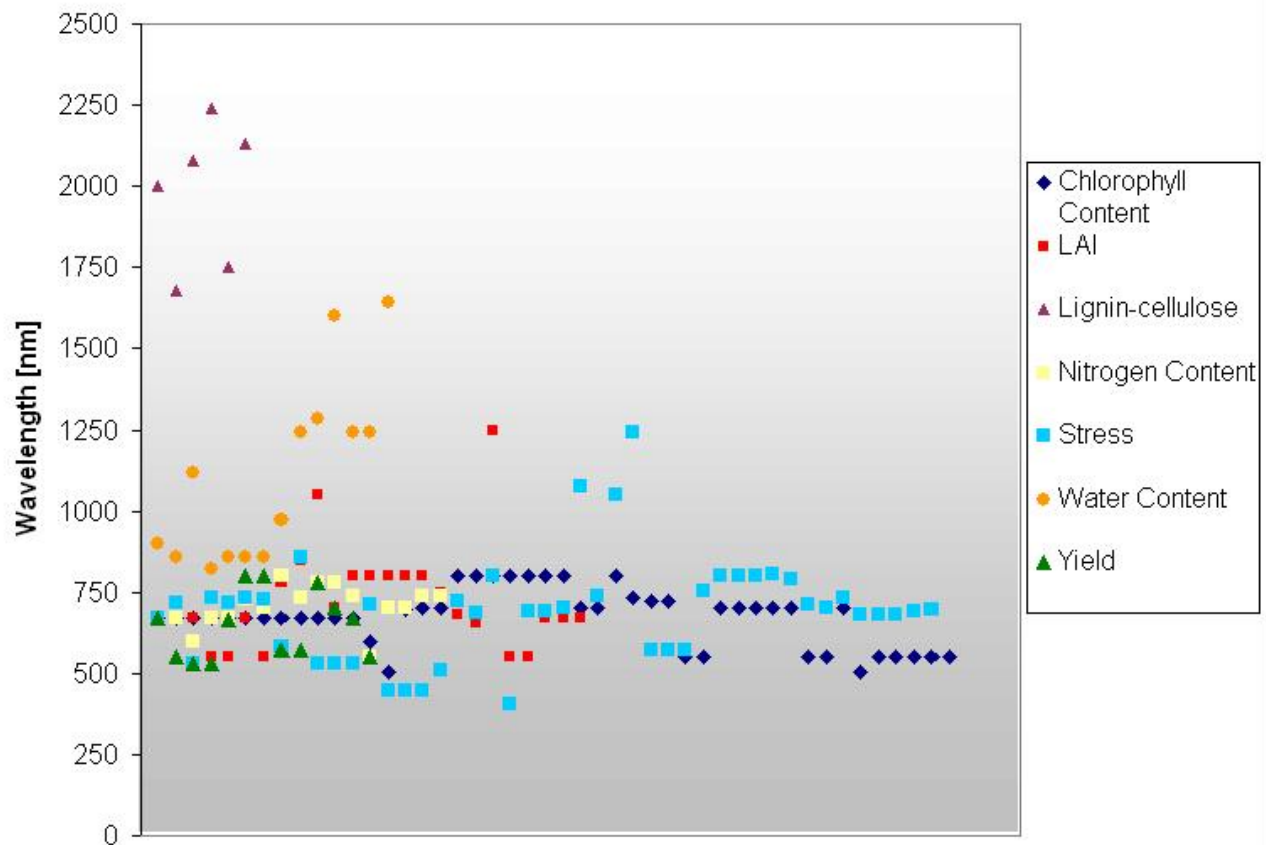


Figure 6: Distribution of index bands used for the determination of biophysical parameters in agriculture

Water content retrievals use index approaches at wavelengths located in the water absorption bands around 850-860 nm, 970 nm and around 1240 nm as shown in Figure 6. On canopy level, indices that are ranged in these weaker liquid water absorption bands appeared to be better water content predictors than those ranged at longer wavelengths at 1600 nm. For the detection of biochemical components (Lignin, Cellulose) the shortwave infrared wavelength region has been proven most suitable. Most studies concerned with stress detection are descriptive experiments using a wide set of spectral bands. Observation of solar-induced fluorescence at 760 nm offers good potential for stress detection; however, more research in this relatively new field has to be conducted. Maturity, phenology, dry matter and yield can only be related indirectly to indices that describe other plant biophysical and biochemical attributes. Therefore they are not contained in Figure 6.

Concluding it becomes evident that the indices use a wide spectral range and hyperspectral measurements are required to allow their acquisition. The graph in Figure 6 might give the impression that the SWIR bands are only of minor relevance, even though mandatory for the retrieval of biochemical components. However in this respect the analysis might be biased, since hyperspectral sensors in this wavelength region are still very rare. That explains why research in this spectral range is not so bulked. Certainly ENMAP's SWIR bands will open up new research areas in agriculture.

In the following for each of the crop parameters a review of recent research results is presented.

2.3. Derivation of Leaf Area Index

The Leaf Area Index (LAI) is defined as “total one-sided leaf area per unit ground”. Because of the role of green leaves in controlling many biological processes in plant canopies it characterizes the structure and the functioning of vegetation. LAI is also a key parameter for precision farming including crop monitoring, prediction of crop growth and yield estimations (Bach et al. 2003, Darvishzadeh et al. 2008, and Garrigues et al. 2008). As LAI is functionally linked to the canopy spectral reflectance, it can be derived from remote sensing data. Benefits and improvements in the estimation of LAI with hyperspectral compared to multispectral data are expected in:

the elimination of soil background and atmospheric effects (Broge and Leblanc 2000),
the differentiation of competing influences of biochemical properties (e.g. chlorophyll) on canopy reflectance (Delalieux et al. 2008, Haboudane et al. 2004) and
the saturation of vegetation indices for high LAI values; depending on the type of vegetation index, a saturation level is approached asymptotically when LAI exceeds 2 to 5 (Haboudane et al. 2004)

A lot of recent studies concentrate on solutions to the interference problem caused mainly by chlorophyll effects and the saturation problem for high LAI values. Due to the fact that LAI and chlorophyll content have connected effects on canopy reflectance from the green (~ 550 nm) to the red-edge (~ 750 nm) region of the electromagnetic spectrum, spectral indices based on the red and NIR spectral features are likely to overestimate the LAI when used on canopies with high chlorophyll content while they are likely to underestimate the LAI of low chlorophyll canopies (Delalieux et al. 2008).

A comparison of the performance of **several indices** that have been analysed and improved for minimizing the effects of leaf chlorophyll has been carried out by Haboudane et al. (2004). They investigated different crop types (soybean, corn, and wheat), at different growth stages, and under different fertilization treatments using both simulated and airborne data. Results determined the indices MTVI2 (Modified Triangular Vegetation Index 2) and MCARI2 (Modified Chlorophyll Absorption Ratio Index 2), both improved variants of the spectral indices TVI and MCARI developed in the context of their study, as best estimators of green LAI. MTVI2 has also been used successfully for LAI estimation of corn, wheat and soybeans by Hu et al. (2004).

Several studies successfully use narrow-band versions of broadband indices, such as the NDVI, RVI and SAVI. Ray et al. (2006) found good correlation between NDVI with the spectral bands 680 and 780 and LAI measurements for potatoes. Lee et al. (2004) successfully applied the spectral bands 655 and 846 nm for a range of vegetation types. They further concluded using canonical correlation analysis that spectral bands located in the red-edge and SWIR regions seem to be more suitable for the prediction of LAI than those located in the NIR.

An increasing number of studies use **Radiative Transfer Models** in the forward mode for reflectance simulation to test the robustness and applicability of indices (Broge and Mortensen 2000, Delalieux et al. 2008, Haboudane et al. 2004). For the estimation of LAI on

a physical basis the dominant strategy in recent years has become the inversion of Radiative Transfer Models. Advantages of the modelling approach include the physical insight into system behaviour and the transferability to different conditions.

For LAI retrieval most studies (> 90%) use a combination of the leaf reflectance model PROSPECT with the canopy reflectance model SAIL (Combal et al. 2002, Darvishzadeh et al. 2008, Koetz et al. 2005, Kamallesh et al. 2008, Meroni et al. 2004) or extended versions of SAIL such as SAILH (Atzberger et al. 2003, 2004, Dorigo et al. 2007) or SLC (Begiebing et al. 2004, Begiebing et al. 2005, Begiebing et al. 2006, Bach et al. 2005, Bach and Begiebing 2007). A combination of PROSPECT with ACRM is used by Kurz et al. (2005) and Houborg et al. (2007).

For model inversion, literature research revealed a favour for neural networks (NNT) and Look-up-table (LUT) approaches. In a comparative study, Combal et al. (2002) concluded that LUT and Quasi-Newton Algorithm (QNT) are very sensitive to modelling errors. NNT overpassed LUT and QNT when model uncertainties are taken into account.

There is good agreement in recent research that, in order to solve the ill-posed problem in model inversion, some sort of regularization is needed. Some authors suggest the introduction of additional spectral constraints (Atzberger 2004), others favour the use of prior information (Combal et al. 2002, Koetz et al. 2005) such as the coupling of the radiative transfer model with a canopy structure dynamics model (Koetz et al. 2005) or a crop growth model (Verhoef and Bach 2003) in order to gain additional information on canopy structure dynamics for the constriction of parameters ranges. Dorigo et al. (2007) use an image-based automated approach to define prior estimates.

Limitations in the use of the leaf reflectance model PROSPECT are seen in the neglect of the optical effects of crop flowering (e.g. for wheat) (Bach et al. 2005, Haboudane et al. 2004), which may lead to an underestimation of LAI. Problems in the simulation of canopy reflectance with PROSPECT and SAIL have been encountered, due to the fact that the turbid medium assumption used in PROSPECT-SAIL does not account for heterogeneities in the canopies (Darvishzadeh et al. 2008, Meroni et al. 2004). This is partly already solved with SAILH where also the hot spot is effect is simulated. The SLC-model (Verhoef and Bach 2007) overcomes both limitations.

2.4. Derivation of Leaf Chlorophyll Content

Being responsible for the process of photosynthesis, the chlorophylls are essential pigments of plant biomass production. The detection of chlorophyll concentration and the relative proportions of chlorophyll a and b, can contribute to a characterization of crop condition. Figure 7 shows the absorption spectra of the major plant pigments. The fact that the spectral absorbance properties of chlorophyll are apparent in the reflectance spectra of leaves offers the opportunity of using hyperspectral measurements as a non-destructive method for quantifying chlorophyll concentration in plants (Blackburn 2007).

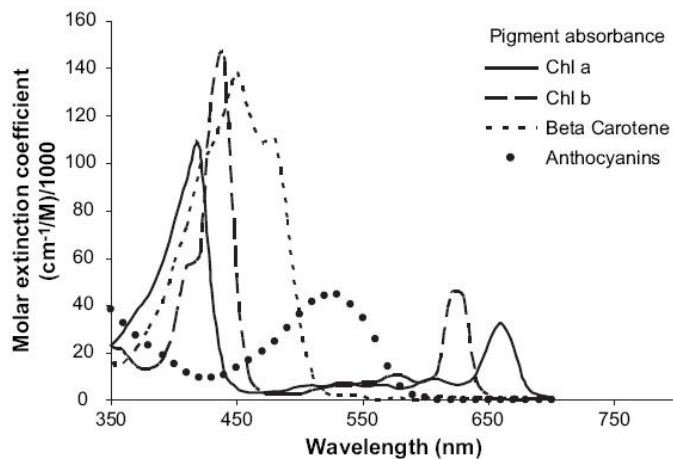


Figure 7: Absorption spectra of the major plant pigments (Blackburn 2007)

In modelling studies there is a good consensus that reflectance is more sensitive to high concentrations of chlorophyll at wavelengths where absorption coefficients of pigments are low, while spectral regions with high absorption show more sensitivity to lower pigment concentrations (Blackburn 2007). Empirical evidence has shown that reflectance at wavelengths at 530-630 nm and 700-750 nm (corresponding to the lower and upper flanks of chlorophyll absorption as can be seen in Figure 7), is most sensitive to normal-range chlorophyll concentrations (Buscaglia and Varco 2002, Carter and Knapp 2001, Sims and Gamon 2002, Strachan et al. 2002, Zhao et al. 2003), whereas low concentrations of chlorophyll, as found in immature and senescent leaves, can be best detected at wavelengths corresponding to the centre of the major absorption features i.e. 660-680 nm (Blackburn 2007, Sari et al. 2005, Sims and Gamon 2002).

A lot of analytical studies are using reflectance in multiple wavebands, in form of **spectral indices** that employ ratios of narrow wavebands in pigment-sensitive and non-sensitive areas to cope with other effects that control leaf reflectance (e.g. leaf structure or leaf surface interactions). A comprehensive listing of chlorophyll spectral indices (state: 2002) has been published by Le Maire et al. (2004). A list addressing all crop parameters is provided in Appendix 1 (Chapter 12). General problems of leaf chlorophyll estimation for agricultural crops based on index-approaches lie in the insensitivity of most indices for low and high chlorophyll contents. It is reported that indices like OSAVI and NDVI become saturated at chlorophyll contents below 0.3 g m^{-2} and above 1.5 g m^{-2} (Oppelt and Mauser 2004). Other difficulties lie in the elimination of non-photosynthetic materials and the correlation to LAI. Addressing the above mentioned issues, a lot of recent studies are trying to improve existing indices (Daughtry et al. 2000, Haboudane et al. 2002).

A widely used index is MCARI (Daughtry et al. 2000), a measure of the depth of chlorophyll absorption at 670 nm relative to the reflectance at 550 and 700 nm. With the implementation of the ratio, the combined effects of the soil reflectance and of canopy non-photosynthetic materials have been reduced. However, MCARI turned out to be still sensitive to background reflectance properties, which causes interpretation difficulties at low LAI values (Daughtry et al., 2000, Haboudane 2004). Another variant of MCARI is TCARI (Transformed Chlorophyll Absorption in Reflectance Index) proposed by Haboudane et al. (2002) for the estimation of

crop chlorophyll content. In TCARI the ratio ($R700/R670$) is used to counteract the background influence only on the reflectance difference ($R700-R550$).

For the prediction of crop chlorophyll content, recent studies suggest combinations of OSAVI and MCARI or TCARI for the estimation of leaf chlorophyll, which provides a solution to LAI correlation and background reflectance effects. The combination MCARI/OSAVI is used by Daughtry et al. (2000) for corn leaf chlorophyll estimation and by Zarco-Tejada et al. (2003, 2004) for open canopy crops (olive trees and vineyards). Haboudane et al. (2002) prefers a combination of TCARI/OSAVI for the estimation of corn leaf chlorophyll content, arguing with the increased sensitivity of TCARI to low chlorophyll values and its greater resistance to vegetation non-photosynthetic materials. TCARI/OSAVI has also been used successfully for the retrieval of chlorophyll content of corn, soybeans and wheat by Hu et al. (2004) and for wheat by Oppelt et al. (2007). Results from Zarco-Tejada et al. (2004, 2005) demonstrate good results for the combined indices TCARI/OSAVI and MCARI/OSAVI for open canopy crops, and poor performance of traditional indices such as NDVI, SR or MSR.

For tracking of leaf chlorophyll content throughout a whole cropping cycle of wheat and barley, indices located in the visible and near-infrared wavelength region (PSSR, TCARI/OSAVI) have not proven successful (Kneubühler 2002). The limitation of spectral indices becomes thus visible.

Studies focusing on the generality of chlorophyll indices through testing and refinement over a range of physiological conditions and species were carried out by Sims and Gamon (2002), and Le Maire et al. (2004). Both studies agree that effect of differing leaf surface reflectance has important influence on index generality. To avoid the effect of differences in leaf spectral reflectance (specular effect as opposed to internal component effect), a modification using a “base wavelength” is introduced, which significantly improves leaf level results. Best results were achieved with the modified indices mSR and mND ($(R750-R705)/(R750+R705-2R445)$, $(R750-R445)/(R705-R445)$ respectively (Le Maire et al. 2004, Sims and Gamon 2002). A similar index has been developed by Datt (2003), who used R680 instead of R445.

A different technique, with improved sensitivity for low and high chlorophyll concentrations, which is based on spectral envelope measurements, is suggested by Oppelt and Mauser (2001). With the Chlorophyll Absorption Integral (CAI) the leaf chlorophyll content can be determined through measuring the area between a straight line connecting two points of the red edge and the curve of the red edge itself. It has been successfully tested with airborne hyperspectral data on maize (Oppelt 2002), wheat (Oppelt 2002, Oppelt and Mauser 2004, Oppelt et al. 2007) and grassland (Oppelt 2002).

A number of studies that focus on the relationship between the red edge (λ_{RE}) and total chlorophyll concentration (CHL tot) use derivatives of the original reflectance spectra to define the wavelength position of the red edge (λ_{RE}). Advantages of using derivatives over spectral reflectance were seen in their ability to reduce variability due to changes in soil/litter reflectance or illumination (Dawson and Curran 1998, Blackburn 2007). Limitations of this approach lie in the existence of two or more peaks in the first derivative spectra in the region of the red edge, which can result in a bimodal distribution of λ_{RE} values corresponding to low and high chlorophyll concentrations.

A more generic approach to quantify leaf chlorophyll content is offered through the use of **Radiative Transfer models**. In forward mode they have been frequently used for the identification of spectral variables or indices that are suitable for the estimation of chlorophyll concentration (Daughtry et al. 2000, Haboudane 2002, Zarco-Tejada et al. 2003, Zarco-Tejada et al. 2004, Zarco-Tejada et al. 2005). Blackburn and Ferwerda (2008) use leaf-scale radiative transfer models for the generation of large spectral data sets with which they developed and tested the application of wavelet analysis for the prediction of chlorophyll estimations. Results showed that the wavelet-based approach outperformed several common indices.

Experimental studies in the inverse mode using the leaf reflectance models PROSPECT and LEAFMOD were conducted by Jacquemoud et al. (1996), Ganapol et al. (1998) and Renzullo et al. (2006). On canopy level, chlorophyll content has been estimated using coupled leaf and canopy models in inverse mode (Begiebing et al. 2005, Combal et al. 2002, Jacquemoud et al. 2000, Zarco-Tejada 2002). Improvement has been achieved by using models that explicitly consider canopy heterogeneities such as vertical leaf colour gradient and clumping effects (e.g. Verhoef and Bach, 2007).

2.4.1. Chlorophyll Fluorescence

Fluorescence is a process by which the light energy absorbed at one wavelength is re-emitted at a longer wavelength because excited electrons return to the lower energy state. Chlorophyll fluorescence (CF) is emitted in two broad bands with peaks at 685 nm and around 740 nm (Rascher and Pieruschka 2008). The fluorescence signal can be used in order to check on the vitality of the photosynthetic apparatus. Generally, steady-state chlorophyll fluorescence and photosynthetic rates are inversely related, which means that **fluorescence is low when photosynthesis is high**.

The fluorescence flux can be detected passively in very narrow dark lines of the spectrum in which solar incident irradiance is strongly reduced (Fraunhofer lines). At 760nm, for example, terrestrial atmospheric molecular oxygen strongly absorbs incoming solar light and the resulting incident radiation at ground level is significantly reduced with respect to the surrounding continuum (up to more than 90% of attenuation). In such dark lines, fluorescence can be detected by measuring to what extent the “wells” are filled by fluorescence relative to the continuum (Meroni et al. 2006). This technique forms the basis of the Fraunhofer line depth (FLD) principle that has recently been improved by Alonso et al. (2008).

Several studies have been concerned with the effects of chlorophyll fluorescence (Meroni et al. 2006, Zarco-Tejada et al. 2003 and Zarco-Tejada et al. 2002). Van der Tol et al. (2009) who have developed a leaf biochemical model for steady-state chlorophyll fluorescence and photosynthesis, describe chlorophyll fluorescence as „the most direct measure for instantaneous vegetation growth that is currently available for remote sensing“. Several campaigns are currently carried out in the fluorescence explorer (FLEX) – mission to evaluate the accuracy with which sun induced fluorescence can be used to quantify photosynthetic efficiency and stresses (see e.g. http://www.esa.int/esaLP/SEMQACHYX3F_index_0.html).

Whether the spectral resolution of ENMAP (~6 nm at the oxygen absorption band) will allow a quantitative retrieval of fluorescence still needs to be studied in detail. Certainly the retrieval needs to account for atmospheric effects. Thus combined simulations with atmospheric radiative transfer will be required as demonstrated by Guanter et al. (2007).

2.4.2. Estimation of Nitrogen Content (leaf level/canopy level)

Nitrogen (N) is the most limiting factor in crop growth in humid regions and the knowledge of nitrogen content of crops is of great importance for agricultural management practices, especially in precision farming. The current N-content of the crop provides information on the nutritional supply of the plants and the expected quality of the yield products (Jarmer et al. 2003, Li et al. 2008, and Zhao et al. 2003). A sufficient supply of N to crops is fundamental for yield optimization. However, mismanagement of N, resulting in over fertilization is ecologically and economically not desirable. Efficient monitoring of crop N status and adequate N fertilizer management are therefore important measures to ensure yield optimization while keeping fertilizer costs and environmental damage (especially water quality loss) as low as possible (Jain et al. 2007, Oppelt and Mauser 2004). An estimation of N in the laboratory is expensive, time consuming and difficult to manage during the crop growing cycle, which makes an estimation of nitrogen content by means of remote sensing devices desirable.

In the last decades a lot of research has been carried out using spectrometer data and statistical methods for the assessment of suitable wavelengths for N content determination. Results show, that nearly the complete reflective domain in the visible (except between 400–490 nm), NIR and SWIR region contains information about leaf nitrogen content (Jarmer et al. 2003, Jain et al. 2007). Areas of interest can be found around 550 nm (Buscaglia and Varco 2002, Jarmer et al. 2003, Strachan et al. 2002, Zhao et al. 2003) in the red edge region (between 600-780) (Buscaglia and Varco 2002, Cohen et al. 2007, Ferwerda et al. 2005, Jain et al. 2007, Mistele and Schmidhalter 2008, Oppelt and Mauser 2004, Zhao et al. 2003) and in the SWIR region (1000-1500nm) (Jarmer et al. 2003, Serrano et al. 2002), 1980 nm (Huang et al. 2004), 2054 nm (Kokaly 2001), 2075 nm (Johnson 2001) and between 2130 nm to 2180 nm (Huang et al. 2004, Johnson 2001, Kokaly 2001).

In the visible region, nitrogen itself does not absorb or reflect directly, but is correlated with the chlorophyll content (Oppelt and Mauser 2004). Oppelt and Mauser (2004) report that the estimation of leaf level nitrogen based on the correlation with chlorophyll content in the VIS/NIR region faces two difficulties:

1. the saturation of a lot of indices or ratios at high chlorophyll contents
2. a reduced chlorophyll-nitrogen correlation at high N availability due to “luxury” N consumption of plants.

At leaf scale, index approaches related to chlorophyll content seem to have a relatively weak correlation with nitrogen content especially at the beginning of the growing season (Buscaglia and Varco 2002, Cohen et al. 2007, Ferwerda et al. 2005, Jain et al. 2007, Mistele and Schmidhalter 2008, Oppelt and Mauser 2004, Serrano 2002) and for ripening

vegetation (Serrano et al. 2002). Promising results for estimating foliage nitrogen concentration are presented by Huang et al. (2004) using continuum removal analysis and HyMap data.

Results for the canopy level show higher correlation coefficients throughout the whole vegetation period (Mistele and Schmidhalter 2008, Oppelt and Mauser 2004). Mistele and Schmidhalter describe high correlations for the Red Edge Inflection Point (REIP) index and Nitrogen Nutrition Index (which describes the relationship between actual canopy N and critical canopy N), attesting the capacity of REIP as a useful measure for the support of N fertilizer application. Similar conclusions are drawn by Stickse et al. (2004), who investigated the sensitivity of several indices to varying N rates in winter wheat in the course of a day. The two indices least affected by diurnal variations and most sensitive to the nitrogen induced heterogeneities were REIP and the Infrared Index (IRI).

2.5. Estimation of Plant Water Content (leaf level/canopy level)

For optimal plant development a balanced water supply is important. Therefore, the accurate quantification of plant water content is a crucial issue for agricultural management especially in arid regions.

The main parameter that describes the amount of water in vegetation in context of remote sensing is the leaf equivalent water thickness (EWT, g/cm²), defined as “depth of liquid water/area” (Cheng et al. 2006). At the canopy level, the canopy water content (CWC) can be defined as the quantity of water per unit area of ground surface (g/m²). The estimation of these parameters by means of hyperspectral remote sensing techniques is possible because liquid water strongly absorbs solar radiation throughout the near-infrared (720–1000 nm) and short-infrared (1000–2500nm) spectral regions. Reflectance is reduced to a varying extent within the water absorption features centred on 970nm, 1200nm, 1450nm, 1530nm, 1720 nm, 1940nm, and 2500 nm, which can be detected and quantified as water content variations (Sims and Gamon 2003, Ustin et al. 2004). Figure 8 shows the water absorption coefficients and canopy reflectance as a function of wavelength.

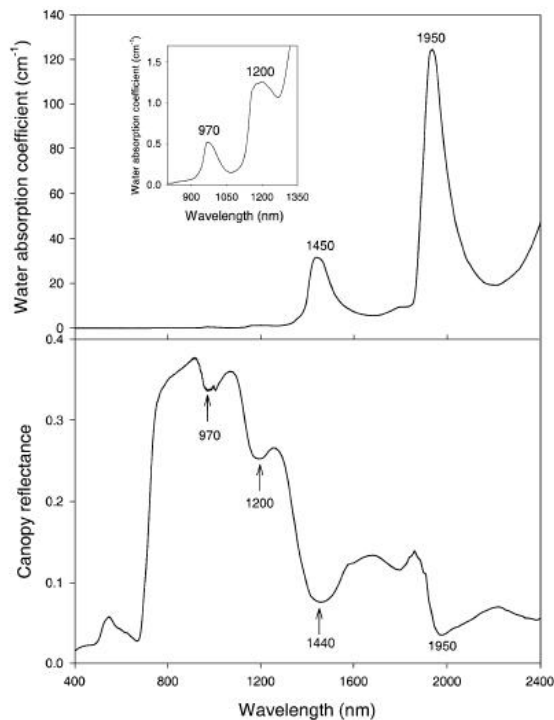


Figure 8: Water absorption coefficients and canopy reflectance as a function of wavelength (Sims and Gamon 2003).

On leaf level good results were achieved with indices in the 1200nm region based on **continuum removal techniques** for the retrieval of leaf water content (Pu et al. 2003). Figure 9 illustrates the continuum removal technique and the definitions of three absorption features. The continuum removal technique has the advantage of standardizing the overall level of reflectance and minimizing the influence of variation in internal leaf structure on the relative area of the absorption feature at 1200 nm. Leaf level study results indicate that the use of SWIR bands alone is unsuitable for successful EWT retrieval, as internal structure and dry matter also influence leaf reflectance, so that a combination of SWIR and NIR is recommended.

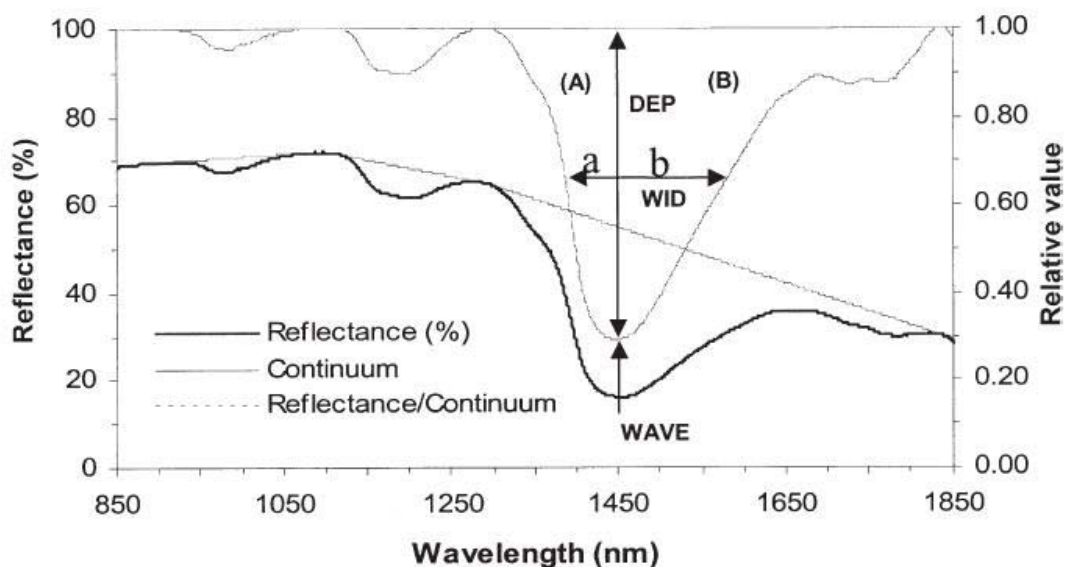


Figure 9: Leaf reflectance spectrum adjusted by a continuum removal technique and the definitions of three water absorption features (Pu et al. 2003).

On canopy level, indices that are ranged in the weak liquid water absorption bands around 850-860 nm, 970 nm and around 1240 nm (i.e. NDWI, SRWI, WI) are better water content predictors than those ranged in longer wavelengths at 1600 or 2220 nm (i.e. MSI, NDII, DWI). This is especially observed for high vegetation cover and can be explained by the greater penetration of radiation within the canopy and the lower saturation at the weaker water absorption bands at these wavelengths (Behrens et al. 2006, Sims and Gamon 2003, Sonnenschein et al. 2005).

Several studies use a spectrum matching technique implemented in the MODTRAN-based radiative transfer model ACORN (ACORN, ImSpec LLC, Analytical Imaging and Geophysics LLC, Boulder, CO) (Green et al. 1991) developed to simultaneously estimate water vapour and liquid water (Trombetti et al. 2008). ACORN is commercially distributed. The technique was originally developed to improve water vapour retrieval from AVIRIS data by fitting measured radiance centred at 940 nm to a radiance spectrum of water vapour absorption generated by ACORN. Due to a spectral difference of 40nm between the centre wavelength of liquid water absorption and water vapour absorption, the simultaneous retrieval of liquid water and water vapour is possible by fitting the measured pixel reflectance to the equivalent transmittance spectrum for a slab of water based on the Beer-Lambert Law (Green et al. 1993, Cheng et al. 2006). Results using ACORN proved good sensitivity to EWT and CWC, except for crops with dense stems e.g. corn (Champagne et al. 2003). Difficulties in EWT estimation include errors due to soil background reflectance and moist residue cover (Cheng et al. 2006, Champagne et al. 2003). Poor results were achieved for within-crop EWT estimation during the early stages of plant growth for wheat (Champagne et al. 2003).

2.6. Derivation of Biochemical Components (Cellulose, Lignin)

Plant biochemical composition can be related to factors that control plant growth and decomposition. Foliar lignin and cellulose concentration is related to litter decomposition rates, which in turn have influence on the flow of nutrients, carbon, water, and energy in terrestrial ecosystems (Serrano et al. 2002). The quantification of plant litter cover on the soil surface is necessary in agricultural systems for the evaluation of the conservation tillage practices which protect soils from erosion. Crop residue on agricultural soils decreases soil erosion by reducing runoff volumes and nutrient removal. It also has effects on soil physical and chemical parameters including water infiltration, evaporation, porosity and soil temperatures. Left on agricultural soils, it improves soil structure, facilitates tilling and influences fertilization regimes (Nagler et al. 2003).

Plant litter and soil do not have unique spectral features in the VIS-NIR and may differ only in their amplitude at a given wavelength. For the distinction of litter from soils, the shortwave infrared wavelength region has been proved suitable for accurate quantification of litter (Daughtry 2001, Nagler et al. 2003). Based on laboratory measurements of dried and ground plant foliage, a lingo-cellulose absorption has been located at 2100nm (see Figure 10) and an index has been proposed by Daughtry 2001: the cellulose absorption index (CAI; not to be confused with Chlorophyll Absorption Integral, which is also called CAI) based on the reflectance in three 50-nm-wide bands—two on the shoulders at 2021 and 2213 nm and one

at 2100 nm (cellulose–lignin absorption max.). Studies using CAI showed significant correlation with percent residue cover for a variety of agricultural crops (Nagler et al. 2003).

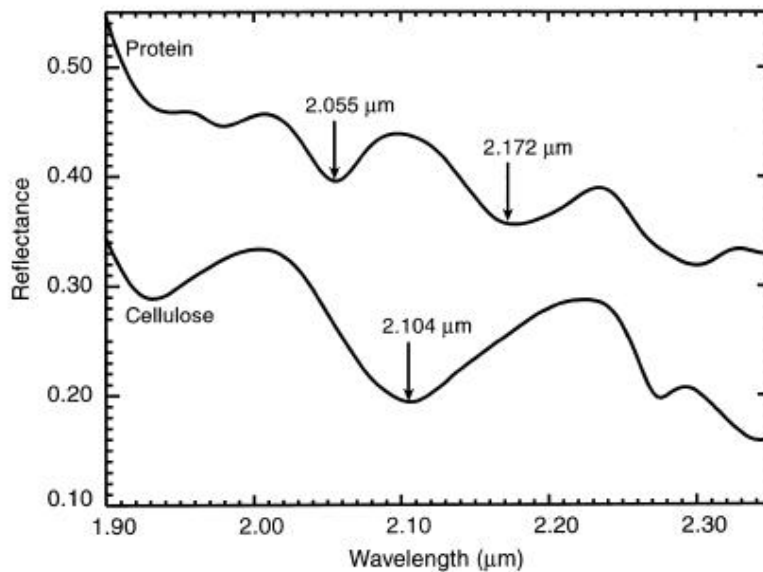


Figure 10: Reflectance spectra of leaf constituents: protein (vegetable protein in powder form) and cellulose (100% cotton-bond paper). The protein spectrum shows two absorptions at 2.055 μm and 2.172 μm , which lie on the shoulders of the broad 2.104- μm absorption feature of cellulose (Kokaly 2001)

Serrano et al. (2002) uses the Normalized Difference Lignin Index (NDLI) for the estimation of bulk canopy lignin, derived from reflectance at 1750nm. Results are satisfying except for ripening vegetation or low vegetation covers, where a lack of correlation between NDLI and the foliar and bulk canopy lignin has been observed.

2.7. Determination of Maturity and Phenology

Crop phenology monitoring is required for the understanding of intra and inter-annual variations of agro-ecosystems and for the improvement of yield prediction models (Vina et al. 2004, Bort et al. 2005). Crop phenology attributes such as the time of flowering or crop maturity are successfully used in programs aiming at yield optimization (Bort et al. 2005). Information on the phenological stage of crop development is important for time-specific crop management practices, especially during crucial periods (e.g. grain filling in cereal crops or harvest) (Kneubühler 2002).

During a growth cycle a crop passes through a series of development phases: a vegetative phase (Germination, seedling growth and tillering), a generative phase (stem elongation, booting, inflorescence emergence and flowering) and a reproductive phase (different ripening stages) (Kneubühler 2002). Within these stages, there are several transitions of importance in terms of management by producers (Vina et al. 2004):

- crop emergence (date of onset of photosynthetic activity),
- tasseling (date when maximum leaf area is attained and tassels emerge, and
- initiation of senescence (date at which green leaf area visibly begins to decrease).

Maturity and phenology can be related to indices that describe the plant biophysical and biochemical attributes. Kneubühler (2002) has analyzed plant biophysical and biochemical parameters such as LAI, chlorophyll content and water content with respect to their suitability to track the stages of crop development. He concluded that plant water content, followed by LAI, are the key parameters for crop phenology monitoring. The phenological stages of the reproductive phase are characterized by the grain water content, which is important as a maturity and harvest indicator. In this phase grain water content could be successfully correlated to plant water content.

Vina et al. 2004 used Visible A

tmospherically Resistant Index (VARI) in a multitemporal approach for the assessment of crop phenology. VARI showed a linear relationship with green vegetation fraction and higher sensitivity to moderate-to-high green vegetation fraction than NDVI. It also enabled an earlier detection of the onset of senescence and thus bears the potential for early detection of crop stress.

Behrens et al. (2006) observed the key physiological and morphological characteristics and reflectance spectra of canopies of oilseed rape and spring barley during the entire growth period. He concluded that for the entire growth period, common vegetation indices like NDVI and SR showed only weak correlations with growth characteristics. According to Behrens, this can be explained by the fact that indices are substantially reduced during flowering in parts of the VIS bands because canopy reflectance increased in the yellow wavelength bands due to reflectance of yellow flower petals. Better performances were achieved by indices of the NIR bands (R 850, SRWI) for tracking physiological and morphological canopy characteristics.

For the determination of crop maturity with radiative transfer (RT) models, Bach et al. (2006) and Begiebing et al. (2006) used the radiative transfer model SLC and multi-angular observations of CHRIS data for the derivation of average leaf angle distribution in wheat crops. As leaf angles are closely related to the phenological development, the intra-field variability of the maturing process could be mapped. Major improvements in assessing crop maturity and phenology are expected through the combined use of radiative transfer and crop growth models.

2.8. Estimation of Dry Matter and Yield

2.8.1. Yield Estimation

A reliable yield estimation or forecast enables improved planning, management of grain production, handling, and marketing (Dente et al. 2008). An essential component of the successful implementation of precision farming is the creation of yield maps. Remote sensing systems are capable of acquiring information over a large area within a very short period of time, which offers great advantages over harvester-mounted yield monitoring in the creation of yield maps. Furthermore, digital imaging systems can provide real-time information on the condition of the crop and allow estimates of crop yield long before the actual harvesting. Especially the introduction of hyperspectral sensors, with their capability of simultaneously gathering and recording spectral information in hundreds of wavebands, bares the potential to further revolutionize the application of remote sensing in yield estimation. (Uno et al 2005).

For the application of vegetation indices for crop yield estimation the use of a spectral index is questionable. Several studies confirm that the indices NDVI, SR and PRI provide relatively weak relationships with yield (Aparicio et al. 2000, Uno et al. 2005). Various environmental factors such as background effects and crop canopy conditions create “noise” that affects the spectral reflectance on the canopy level. Studies using index approaches showed that there are no stable relationships between indices and yield throughout the whole vegetation period. For example, Gat et al. (2000) concluded that traditional vegetation indices alone may not capture all the required information. Instead he proposed a combination of the time-integrated indices.

Also Zarco-Tejada et al. (2005) tested the most common indices for the estimation of in-field yield variability of cotton. Their results showed that the relationship obtained between vegetation indices and spatial yield data varied over time. The best results were achieved by them during the early growth stages, whereas during later stages less strong relationships resulted. Structural indices related to LAI showed the best relationships with yield at the early growth stages, whereas hyperspectral indices related to crop physiological status (TCARI, MCARI) proved better suited for later growth stages. Good results for the combination of TCARI/OSAVI during early stem elongation of barley were reported by Pettersson et al. (2005) for barley yield estimations. Aparicio et al. (2000) observed significant correlations between the indices and wheat yield in a rain fed environment only at anthesis, in the irrigated environment only at maturity, and only at crop stages with LAI < 2.5.

As a conclusion one can summarise that correlations with different spectral indices can be observed under certain circumstances, but statistical methods do not provide a reliable solution. Since yield, like grains, can not directly be observed with remote sensing, a more complex approach is required to provide yield maps.

This consists of assimilation of for example LAI maps retrieved from EO in crop growth models. Crop growth models simulate the biomass allocation including the forming of grains in the canopy based on environmental factors (rainfall, temperature, soil conditions, etc.). The spatial representation of the current development status of the field is retrieved from optical remote sensing. Through the assimilation of this remotely sensed information in the crop growth model, dry biomass and yield simulation are much closer to observations compared to pure growth model results (Bach and Mauser 2003).

Begiebing et al. (2007) use the SLC model coupled to a crop growth model for the creation of yield maps. Figure 11 illustrates the applied coupling between radiative transfer and crop growth model for spatially distributed retrieval of geo-biophysical parameters. The concept was applied both to multispectral and hyperspectral data. Assuming that the LAI retrieval is improved using hyperspectral data, also improvements of yield estimations using ENMAP like data can be expected.

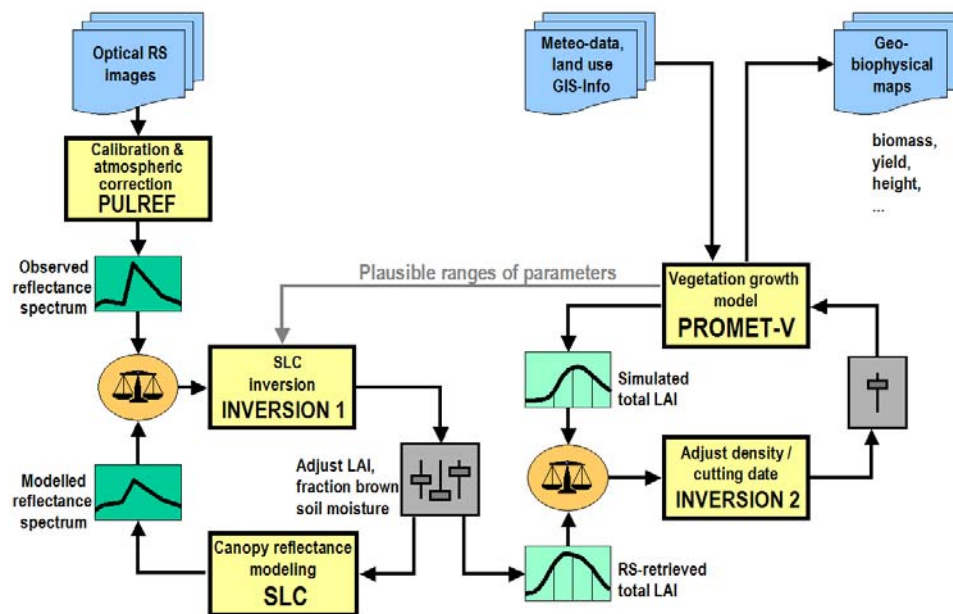


Figure 11: Coupling between radiative transfer and crop growth model for spatially distributed retrieval of geobiophysical parameters, Begiebing et al. 2007 (Adapted from Verhoef and Bach 2003)

2.8.2. Dry Matter Estimation

Accurate estimates of Dry Matter (DM) provide valuable information about the productivity and functioning of agricultural products.

Attempts to retrieve dry matter using statistical approaches give almost the same heterogeneous picture as for yield: Clark et al. (2003) proposed to use a carbohydrate/lipid CH absorbance band around 900-920nm as the most important band for DM estimation as it is free from interferences of the water absorbance bands that typically dominate plant spectra. Aparicio et al. (2000) tested several common indices (SR, NDVI, PRI) for their potential of dry matter estimation in wheat. They found positive correlations of dry matter with SR and NDVI only at milk-grain stage in an irrigated environment and at physiological maturity in a rain-fed environment. PRI showed positive correlations with DM only at physiological maturity under irrigation. Cho et al. (2007) showed good results for biomass estimation of grass using PLS regression involving continuum-removed bands. Clark et al. (2003) and Biewer et al. (2008) tested various statistical techniques for the prediction of dry matter, where PLS (Partial Least Squares) gained better results than MLR (Multiple Linear Regression).

As conclusion there is no agreement in recent literature on an index approach that enables a stable relationship between an index and dry matter throughout the growing season. For the estimation of dry matter however again the assimilation of crop parameters like green LAI or FAPAR in a crop growth model is recommended. This is demonstrated by Bach & Mauser (2003) and Bach et al. (2000).

2.9. Crop Damage and Stress Detection with Hyperspectral Data

Plant stress can be caused either by nutritional shortage (mainly due to water or nitrogen deficits) or due to other environmental factors such as pest infection or temperature stress. Early detection of plant stress is of growing importance in the framework of precision farming applications. The targeted use of pesticides could decrease potential risks to the environment and ecosystem, and also lower the cost of application. Spectral reflectance analyses have proven to be very useful in detecting plant stress due to changes in the absorption of incident light in various wavelength regions of the electromagnetic spectrum. The high spatial and spectral resolution of hyperspectral technology increases the potential to detect anomalies in the normal plant production processes at an early stage, thereby providing accurate means to model and monitor plant production systems. This is especially important for capital-intensive perennial crops, such as fruit species (Delalieux et al. 2007).

2.9.1. Nitrogen Stress

The identification of nitrogen stress in a crop is crucial for site-specific fertilizer management as plant nitrogen (N) deficiency often limits crop productivity. A lot of studies have been carried out using statistical techniques for the identification of the optimum bands and also narrow-band indices for crop N stress assessment (Meuleman et al. 2003, Erasmi and Kappa 2003, Perry et al. 2000, Strachan et al. 2002). Most of the studies were carried out using portable spectrometer data (Jain et al. 2007, Jorgensen et al. 2007, Tilling et al. 2007, Zhao et al. 2003, Zhao et al. 2005). In the visible region (550-680 nm) of the spectrum N-stress can be detected since nitrogen is one of the basic compound molecules of chlorophyll (Meuleman et al. 2003). In general, N deficiency usually decreases leaf chlorophyll concentration, thus the retrieval of chlorophyll content leads to estimates of nitrogen stress.

2.9.2. Climate – induced Stress (water, temperature, humidity)

When evaporative losses of water exceed the soil water supply, crops are confronted with water stress. The result is a degradation of physiological processes. Even short periods of water stress may result in lower crop yields, so that a detection of water-induced stresses is of great importance for agriculture. Suitable wavelength regions for climate-induced stress detection lie in the VIS-NIR region (Rascher and Pieruschka 2008, Suarez et al. 2008), fluorescence region between 650 and 770 nm (Zarco-Tejada et al. 2003, Dobrowsky et al. 2005), as well as in the thermal region (Sepulcre-Canto et al. 2007).

Zarco-Tejada et al. (2002, 2003) investigated the relationship of chlorophyll fluorescence (CF) and temperature and humidity stress. Under raising stress, plant tissues shift toward increasing heat production to dissipate excess energy, which has the effect of reducing chlorophyll fluorescence at least in the initial and intermediate stages of stress. Through canopy derivative reflectance analysis, short-term and long-term stress was associated with the variation of the fluorescence emission, demonstrating that the double-peak feature at 690–710 nm in the canopy derivative reflectance is directly related to the natural fluorescence.

Dobrowsky et al. (2005) used the fluorescence ratio indices (FRI) in order to detect plant stress caused by heat and water. The indices are calculated from wavelengths affected by fluorescence emission (650 - 770 nm with emission peaks at 690 nm and 740 nm) that are normalized by wavelengths not affected by CF emission (e.g. 600 nm, 800 nm).

2.9.3. Biotic Stress (Infectious Stress)

Disease infection is one of the major factors threatening sustainability of agricultural production, which makes detecting biotic stress an important issue. The proper characterization and assessment of disease distribution and severity in near-real-time could provide useful information for making decisions regarding the application of fungicide not only when but also where necessary in precise agriculture management (Liu et al. 2008).

Biotic stress (e.g. caused by infection with plant pathogens), generally affects the chlorophyll absorption of photosynthetic active radiation leading to an increase of reflectance in the 400 to 700 nm domain (Huang et al. 2007). Breakdown of leaf, e.g. necrosis caused by pathogens, results in loss of leaf area, decreased foliage density and changes in leaf orientation, which decreases the reflectance in the near infrared (Larsole and Muhammed 2007, Mirik et al. 2007). A study carried out by Carter and Knapp (2001) showed that maximum difference in reflectance between healthy and stressed plants occurred near 700 nm. Suitable wavelengths for the detection of biotic stress on apple trees (scab infection) have been found according to Delalieux et al. (2005, 2007) in the 1350–1750 nm region and 2200–2500 nm region for early detection of infection (before the damage is visible) and in the visible spectrum at 580–660 nm and 685–715 nm for later infection stages. These results correspond to the results of Meuleman et al. (2003), who concluded that for the discrimination between stresses (i.e. scab infection and nitrogen stress) the use of wavelength regions in the NIR and SWIR (around 750nm and above 1400nm) is required.

Concluding, biotic stress has very variable appearances in spectral signatures with sensitivities in different spectral ranges depending on the type of biotic stress. A model based approach for biotic stress detection has not been described so far.

2.10. Classification Methods for Agricultural Crop Identification

Maps of crop type are created by national and multinational agricultural agencies, insurance agencies, and regional agricultural boards to prepare an inventory of crops serving purposes such as grain supplies forecasting, collection of crop production statistics, identification of factors influencing crop stress, and assessment of crop damage due to storms and drought. Key activities include identifying the crop types and delineation of their extent. Remote sensing techniques form an efficient instrument in the collection of the required information.

Agricultural crop classification based on hyperspectral data mostly use the same methods as when multispectral data are classified. The most prominent are Maximum Likelihood, Artificial Neural Networks (Moshou et al. 2002), and Decision Tree classification schemes. The Maximum Likelihood classification is widely distributed and provides good results in case training data are well selected. When the spectral dimensionality of the remote sensing data increases, more training data are however required to provide acceptable estimates of the statistical parameters. This means when using hyperspectral data in a Maximum Likelihood classification, that parameter estimation might become inaccurate, if the number of training data pixels is inadequate (Pal and Mather, 2003). Also Oki et al. (2006) showed for hyperspectral data that Maximum Likelihood is not suitable for the classification of agricultural land in areas where the collection of training data is difficult.

In these cases, a decision tree can be used instead, as presented by Spengler et al. (2007). He created a classification algorithm using a decision tree that also allowed the differentiation of vitality status and applied it on HyMap data. Another solution that makes use of spectral libraries is presented by Rao et al. (2007). He received good results with the Spectral Angle Mapper (SAM) classification algorithm for the identification and classification of rice, sugarcane, chilli and cotton crops.

Agricultural classifications differ from other land use classifications in the high temporal dynamics of the observed land surface. While for example build-up area, water or conifer forest look spectrally rather similar during the year, the reflectance of an agricultural field changes within 3-4 months completely from a bare soil spectrum to a vegetation spectrum with increasing leaf area and finally during maturity to a spectrum of dry biomass. In one year even 2 agricultural uses can be observed. This means that, if no ground truth is taken temporally close to the satellite acquisition, supervised classifications are not feasible. Instead, this temporal development must be considered for example by using the phenological development of agricultural crops in the classification.

Having these temporal dynamics in mind, Itzerott and Kaden (2006, 2008) generated an algorithm for crop classification based on 15 years of Landsat TM/ETM data and temporal NDVI indices. The resulting standardized curve connects the phenological state of the crops with the specific spectral information, enabling an identification of crop type on field level. This concept of using temporal trends of crop development can also be applied to hyperspectral data.

Migdall et al. (2009) use a model-based approach where land-use classification is combined with the retrieval of canopy variables. For this, the canopy reflectance model SLC is inverted using a look-up-table approach and the RMS error as decision criterion. The inversion allows for each landuse class only specific ranges of optical parameters that are used in SLC. A priori knowledge about the phenological stage of the crops in the target area at the time of image acquisition is used to constrain the pre-defined parameter space of the inversion. The method is globally applicable to multi- and hyperspectral optical sensors. The model inversion is calculated over all pixels for all defined land-uses. When using only a singular acquisition, the resulting land-use is chosen by taking the land-use with the lowest RMS value in the resulting set of RMS errors. For multi-temporal analyses, a factor is introduced that takes into account how well a particular land-use class can be distinguished at the date of each individual image acquisition. E.g. wheat fields in Europe can be classified well in May and June but not in July after harvest. Contrary, corn fields can be classified well in July or August, because their vegetation period starts later. The results of the individual inversions are combined using this a priori knowledge.

2.11. Priorities and Recommendation for Implementation

Agricultural applications require the provision of a large set of crop parameters, like LAI, chlorophyll or water content, or stress detection (see also Figure 1). This explains why the number of methods for retrieving this information from hyperspectral data is huge. It will

hardly be possible to implement all these algorithms that proved to be valuable within a toolbox for ENMAP. For example, more than 30 hyperspectral indices were selected in the summary table in Appendix 1 (Chapter 12). However, from the set of methods general algorithms can be concluded that are proposed to be implemented in the toolbox.

Although statistical approaches that correlate crop parameters with a hyperspectral index are not generally applicable and transferable, their application is still dominant in scientific agricultural studies (see Figure 5). Accordingly, a tool shall be generated that allows the calculation of these indices on ENMAP images. The literature review did not reveal that certain indices perform better as others under all conditions. Instead it could be observed that the findings varied a lot from study to study. Also, the spectral bands that provided the best regression results are quite different, as could be seen in Figure 6.

Therefore, it is proposed to develop a **generic index calculator** for ENMAP that allows in an interactive way to do **basic arithmetic calculations** on selectable ENMAP bands. Almost all the indices listed in Appendix 1 can be calculated using addition, subtraction, division, multiplication, factorial transformation, exponential function and logarithm. The user of the ENMAP toolbox should be able to create the formula for his preferred index using an interactive tool and this index should then be saved as a script. This allows the user of ENMAP data to create their own portfolio of algorithms that performed best in their applications. Of course it would also be possible to provide standard scripts in the toolbox, like TCARI, OSAVI, or MCARI, that have proven their applicability in a series of studies.

Besides this arithmetic tool, two further spectral analyses should be included in the toolbox. This is first a method for calculating the derivation of the spectrum including the extraction of the extreme values. This allows the identification of the wavelength and the absolute values of a reflectance maximum or minimum, as well as the calculation of the red edge position. The user just selects the spectral range for which the derivation should be calculated. This user selection is also required for the second tool consisting of the calculation of the **convex hull** and the describing parameters of the absorption as illustrated in Figure 9. This convex hull algorithm will surely also be required for geological applications. If it is structured the way that the wavelength of the absorption maxima can be fixed or variable in a selectable spectral range, the tool would be very flexible in its use.

A combination of a **leaf and canopy reflectance model** as illustrated in Figure 3 is further proposed to be made available to the scientific users of ENMAP. It should in a first stage be available in forward mode providing simulated reflectance values for the ENMAP spectral bands. This will support the scientific community in understanding the sensitivity of observational, soil or crop parameters on the signal measured by ENMAP. A server/client application of **SLC** was presented by VISTA as a possible example for such a tool. In a next step an inversion of a radiative transfer model for crop parameter retrieval (at least for LAI, chlorophyll and water content) is proposed to be installed. Since it should be implemented in the toolbox and also allow a fast calculation time, an **artificial neuronal network** is proposed to be used for this. Parameter retrieval is then fast and easy to be applied by the users. However, the training phase of the neuronal network and its dedication to the ENMAP spectral configuration would require additional efforts and developments.

2.12. Appendix 1: Overview of hyperspectral indices used in agriculture

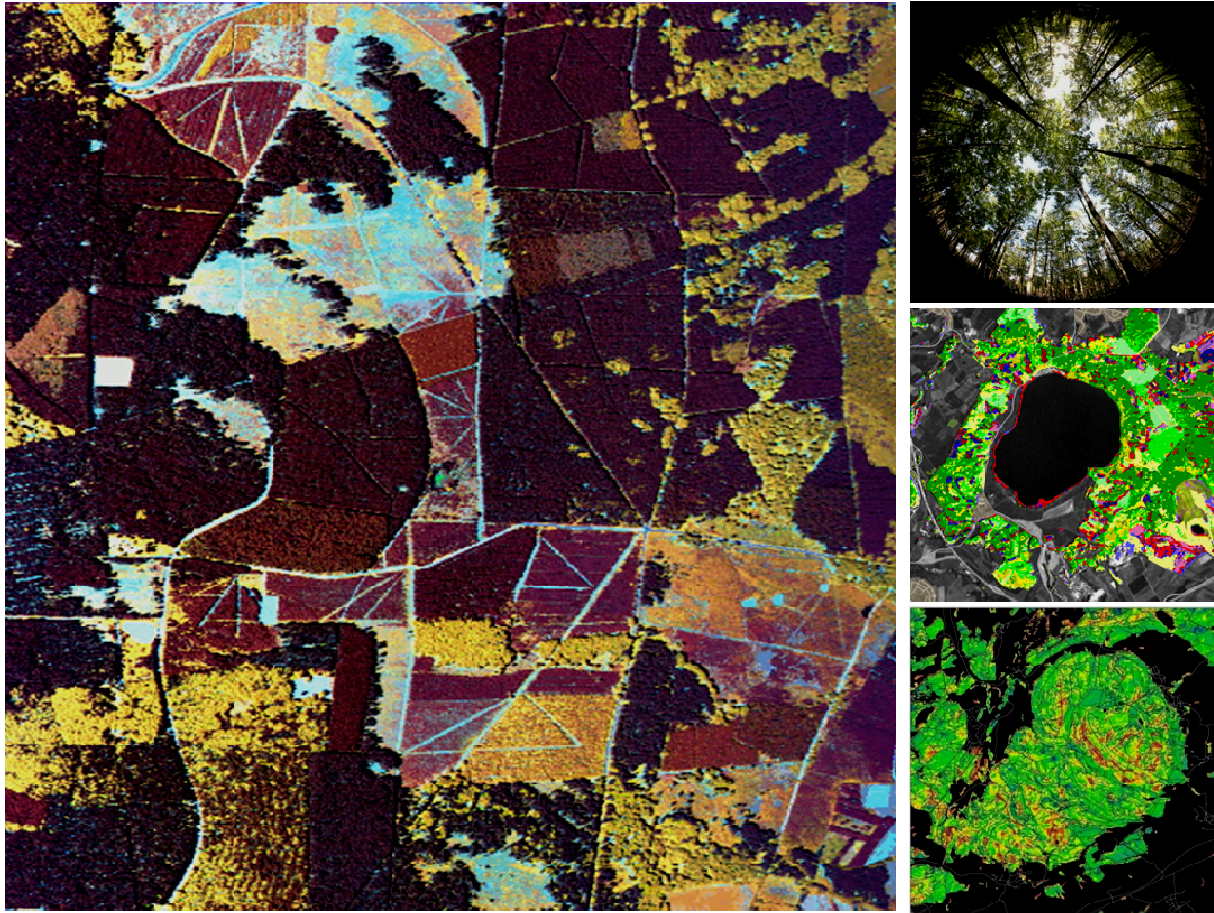
Name	Formula	Used Reflectance at Wavelength [nm]				Author	Investigated Crop	Crop Parameter
		W1	W2	W3	W4			
TCARI	$3[(W2-W1)-0.2(W2-W3)(W2/W1)]$	670 670	700 700	550 550		Haboudane et al. 2002 Zarco-Tejada et al. 2004 Cohen et al 2007	corn olive tress, vineyard potato	Chlorophyll Chlorophyll Nitrogen
OSAVI	$(1+0.16)(W2-W1)/(W2+W1+0.16)$	670 670 670	800 800 800	- - -		Haboudane et al. 2003 Oppelt et al. 2007 Oppelt and Mauser 2003	corn wheat maize and wheat	Chlorophyll Chlorophyll Nitrogen
TCARI/OSAVI		670	800	700	550	Haboudane et al. 2002 Zarco-Tejada et al. 2004 Hu et al. 2004 Kneubühler 2002 Oppelt et al. 2007 Suarez et al. 2008 Pettersson et al. 2005	corn olive tress, vineyard corn,soybean,wheat wheat, barley wheat olive orchard barley	Chlorophyll Chlorophyll Chlorophyll Chlorophyll Stress Yield
MCARI	$[(W2-W1)-0.2(W2-W3)](W2/W1)$	670 670	700 700	550 550	- -	Haboudane et al. 2004 Daughtry et al. 2000 Zarco-Tejada et al. 2004	soybean, corn, wheat corn olive tress, vineyard	LAI Chlorophyll Chlorophyll
MCARI/OSAVI						Daughtry et al. 2001 Zarco-Tejada et al. 2003 Zarco-Tejada et al. 2004	corn olive tress, vineyard olive tress, vineyard	Chlorophyll Chlorophyll Chlorophyll
MCARI2	$1.5[2.5(W2-W1)-1.3(W2-W3)]/WURZEL[(2W2+1)^2-(6W2-5WURZELW1)-0.5]$	670	800	550	-	Haboudane et al. 2004	soybean, corn, wheat	LAI
RDVI	$(W2-W1)/WURZEL(W2+W1)$	670	800	-	-	Haboudane et al. 2004	soybean, corn, wheat	LAI
MTVI2	$1.5[1.2*(W2-W1)-2.5(W3-W1)]/WURZEL[(2W2+1)^2-(6W2-5WURZELW3)-0.5]$	550 550 550	800 800 800	670 670 670	- - -	Haboudane et al. 2004 Hu et al 2004 Zarco-Tejada et al. 2005	soybean, corn, wheat corn,soybean,wheat cotton	LAI LAI Yield
MSAVI	$0.5[2W2+1-WURZEL[(2W2+1)^2-8(W2-W1)]]$	670	800	-	-	Haboudane et al. 2004	soybean, corn, wheat	LAI
TVI	$0.5[120*(W2-W1)-200(W3-W1)]$	550	750	670	-	Haboudane et al. 2004	soybean, corn, wheat	LAI
NDVI	$(W1-W2)/(W1+W2)$	780 846	680 655	- -	- -	Ray et al. 2006 Lee et al. 2004	potato various	LAI LAI
sLAIDI	$S*(W1-W2)/(W1+W2)$ (s=scaling factor equal to 5 to rescale the sLAIDI values)	1050	1250	-	-	Delalieux et al. 2008	Citrus Orchards	LAI

Name	Formula	Used Reflectance at Wavelength [nm]				Author	Investigated Crop	Crop Parameter
		W1	W2	W3	W4			
SAVI	$(1+L)(W2-W1)/(W2+W1+L)$	670	800	-	-	Huete 1988	cotton, grass	Chlorophyll
		663.7	778.2	-	-	Gat et al. 2000	sugar beet	
CAI	normalized convex hull from W1 to W2	600	735	-	-	Oppelt and Mauser 2004	Wheat	Chlorophyll
		600	735	-	-	Oppelt and Mauser 2003	Wheat	Nitrogen
mSR	$(W2-W1)/(W3-W1)$	502	722	701	-	Le Maire et al. 2004	broad leaves	Chlorophyll
mND	$(W2-W1)/(W2+W1-2W3)$	699	722	502	-	Le Maire et al. 2004	broad leaves	Chlorophyll
REIP	$700+40[(W1+W2)/2-W3]/(W4-W3)$	670	780	700	740	Mistele and Schmidhalter 2008	winter wheat	Nitrogen
		670	780	700	740	Stickse et al. 2004	winter wheat	Nitrogen
		670	780	700	740	Behrens et al. 2006	oil seed rape	water content
IRI	$W2/W1$	730	740	-	-	Stickse et al. 2004	winter wheat	Nitrogen
WI	$W1/W2$	900	970	-	-	Sonnenschein et al. 2005	wheat	Water Content
SRWI	$W1/W2$	858	1240	-	-	Behrens et al. 2006	rape and barley	Water Content
	is the area of the absorption feature around 1200 nm obtained by computing the reflectance of the continuum line at wavebands of interest (pCR)							
Acr 1200		1116	1284	-	-	Colombo et al. 2008	poplar trees	Water Content
Simple Ratio	$W2/W1$	820	1600	-	-	Cecatto et al. 2001	various leaves	Water Content
		715	405			Zhao et al. 2005	sorghum	Stress
		530	692			Liu et al. 2008	rice	Stress
		732	692			Liu et al. 2008	rice	Stress
		718	702			Liu et al. 2008	rice	Stress
		735	1075	-	-	Zhao et al. 2005	sorghum	Stress
first derivatives	$[W\lambda - W(\lambda - 1)]/\Delta\lambda$	730	740			Zhao et al. 2005	sorghum	Stress
		580	1050			Erasmí and Kappa (2003)	wheat	Stress
NDWI	$(W1-W2)/(W1+W2)$	860	1240	-	-	Gao et al. 1996	various	Water Content
		858.5	1240	-	-	Cheng et al. 2006	crops	Water Content
		857	1241			Lobell and Asner 2003	wheat	Stress
SIWSI	$(W1-W2)/(W1+W2)$	858.5	1640	-	-	Cheng et al. 2006	crops	Water Content
PRI	$(W2-W1)/(W2+W1)$	531	570	-	-	Suarez et al. 2008	olive orchard	Stress
		531	570	-	-	Perry et al. 2000	corn	Stress
		531	570	-	-	Uno et al. 2005	corn	Yield
		531	570	-	-	Huang et al. 2007	winter wheat	Stress
		531	570	-	-	Ye et al. 2007	citrus orchard	Yield

Name	Formula	Used Reflectance at Wavelength [nm]				Author	Investigated Crop	Crop Parameter
		W1	W2	W3	W4			
RVSI	$(W1+W2)/2-W3$	714	752	733	-	Perry et al. 2000	corn	Stress
CAI	$0.5 \cdot (R2.0 - R2.2) - R2.1$ where R2.0, R2.1, and R2.2 are reflectance factors in bands at 2.00–2.05, 2.08–2.13, and 2.19–2.24 μm	2000	2080	2130	2240	Daughtry et al. 2001 Nagler et al. 2003	corn, wheat and soybean corn, soybean, wheat, r	Lignin-cellulose Lignin-cellulose
NDLI	$[\log(1/W2) \log(1/W1)] / [\log(1/W2) + \log(1/W1)]$	1680	1754	-	-	Serrano et al. 2002	shrub	Lignin-cellulose
VARI green	$(\rho_{\text{green}} - \rho_{\text{red}}) / (\rho_{\text{green}} + \rho_{\text{red}} - \rho_{\text{blue}})$					Vina et al. 2004	maize	Phenology
Red-Green Ratio	$\Sigma(W600 \dots W699) / \Sigma(W500 \dots W599)$					Lobell and Asner 2003	wheat	Stress
SIPI	$(W2 - W1) / (W2 - W3)$	445	800	680		Jain et al. 2007	potato	Stress
		445	800	680		Lobell and Asner 2003	wheat	Stress
		445	800	680		Strachan et al. 2002	corn	Stress
		508.5	804.5	692.5		Mirik et al. 2007	wheat	Stress
CCCI	Calibrated index using NDRE as function of NDVI					Tilling et al. 2007	wheat	Stress
MSRpi	Calibrated index using mSR as function of NDVI					Tilling et al. 2007	wheat	Stress

3. State-of-the-Art and Review of Algorithms with Relevance for Retrieving Biophysical and Structural Information on Forests and Natural Vegetation with Hyperspectral Remote Sensing Systems

Joachim Hill



3.1. Introduction

Remote sensing has been considered a powerful and promising tool for supporting operational forest management as well as forest ecosystem welfare ever since. In fact, information extracted visually from aerial photography is well-understood, accepted, and integrated with field surveys on an almost operational level; ortho-projected photomaps, for example, are routinely used as backdrop for stand allocation maps of the local forest administration in most federal states of Germany, and CIR photos have been extensively used for mapping tree vitality and crown structures in permanent observation sites. Digital remote sensing data acquired by satellite systems, however, is rarely used in forest management.

Reasons might be seen in fact that remote sensing data and digital interpretation methods are complex, and not always well-understood by those who might best use them. Eventually, the technological infrastructure is not in place to make efficient use of the data and, the characteristics of much remote sensing data were, perhaps, not well suited to the problems that have traditionally been of concern to the forest management community. More important, remote sensing (particularly satellite remote sensing) has not been considered a viable information source in the management of the forest because there were always better and less expensive ways of obtaining the necessary information, particularly when the necessary information is limited and narrowly defined (from 1998).

But forest management in Central Europe is changing. Nowadays forest management problems are multiscale and intricately linked to society's needs to measure, preserve, and manage for multiple forest values. Climate change likely creates new pressures upon forests, making their preservation eventually more difficult than expected and imposing new challenges for collecting data and monitoring the state of forests – and all this at a time where financial constraints have led to substantial reduction of staff resources in public forest services; traditional inventories that rely on manpower will soon become the exception. This also creates new challenges for remote sensing: satellite data will not only serve economically-oriented assessments and management needs but be used for studying ecological processes and functions. Derived products will be integrated with other spatial and non-spatial data to form the information base upon which sound forest management decisions can be made (Franklin 2001).

With a focus on both operational forest management and ecosystem functioning this review places major emphasis on the specific strength of hyperspectral imaging systems which are on the verge of becoming operationally available, albeit on commercially operated aircrafts or on research satellites.

3.2. Issues in Hyperspectral Remote Sensing and Sustainable Forest Management

Sustainable forest management supplements a concern with economic values with concerns that species diversity, structure, and the present and future functioning and biological productivity of the ecosystem be maintained or improved (Landsberg and Gower 1996). The changes from an older, traditional forest management approach with an emphasis on timber values to sustainable forest management are profound – a challenging time for considering future directions in forests and forestry (Franklin 2001).

Applications of remote sensing to sustainable forest management are usually presented in four categories that include classification of forest covertype, estimation of forest structure and available resources with regard to more common inventory variables (i.e. tree species, height, age, crown closure), forest change detection and forest modeling. In this perspective, also other variables available by remote sensing, not necessarily in high demand presently for forest management, will be considered because of their potential role in future management scenarios, because in order to better understand their functioning and response to environmental changes, it is necessary to up-scale the available knowledge on stand level to the scale of the entire forest or small region. The distinction between inventory variables and indirect input/output variables of forest productivity models is therefore becoming less relevant because the forest management demand for ecological applications, models and comprehensive forest structure information will continue to grow (Franklin 2001; Landsberg 2003).

In recent times, these forest ecosystems have been exposed to increasing pressure from environmental changes such as global warming and human population growth. The development of adapted management strategies is of utmost importance in this situation (see, for example, www.forestclim.eu/), and with this task and an increasing need to understand the role of forests in the global carbon budget (e.g. Kyoto protocol), forest ecosystems have to be quantitatively analyzed in order to better understand the prevailing processes. The most important processes occurring in forests include carbon exchange (photosynthesis and respiration), evapotranspiration, and nutrient cycling (Waring and Running 2007). Already at the local level, these processes are difficult to measure; at regional to global scales, processes are no longer measurable at all (Tenhunen et al. 1998). Consequently, models have been developed which simulate the fluxes of matter and energy. These simulation models require as inputs (initialization) or for validation purposes accurate estimates of forest structural and chemical properties.

Several studies have demonstrated how remote sensing derived leaf and canopy variables are used to constrain an ecosystem model. Such approaches require spatially continuous inputs on ecosystem state at simulation start and may profit from the assimilation of relevant remote sensing derived biophysical and biochemical state variables (Dufrêne et al. 2005; Kooistra et al. 2008; Le Maire et al. 2005). It has been emphasized that hyperspectral imaging systems allow more detailed and accurate retrieval of relevant vegetation properties (Ollinger and Smith 2005; Schaepman et al. 2004), where the most important vegetation parameters are leaf chlorophyll and nitrogen content, the fractions of photosynthetically

absorbed radiation (fAPAR), canopy water content, annual maximum leaf mass per area (LMA), and annual maximum leaf area (LAI) (e.g. Le Maire et al. 2008).

Forest inventory data for management tasks typically exist as quantitative attributes collected from ground surveys or as forest cover maps interpreted directly from aerial photographs. Survey attributes include tree heights, stem densities, volumes, species, age classes, among others. Traditionally, forest inventories have been repeated every 10 years or longer, and typically exist for forest owned by the state or municipalities, but not for privately owned forest. For instance, in the state of Rhineland-Palatinate about a quarter of the total forest is private (Bundesministerium für Verbraucherschutz, Ernährung und Landwirtschaft, 2004). As private forests may be of great economical and ecological importance, there is a considerable interest of the local and state forest authorities in such inventory data. Consequently, remote sensing approaches capable of mapping important forest attributes such as species type, age class, crown volume and biomass would be of great value.

This review will thus focus on forestry applications where hyperspectral imaging systems are expected to provide a substantial contribution and not on technical aspects, such as the acquisition of imagery, image calibration and processing. Departing from goals and objectives identified under sustainable forest management and ecosystem-based management approaches major emphasis will be placed on the fields of forest classification (forest stand species composition, density, crown closure, height and age), forest structure estimation (continuous variable estimation) and forest change detection (natural disturbances, such as forest damage, defoliation and loss of vitality due to calamities, fire, fragmentation). As specific methods, albeit empirical or model-based, have relevance for different of these contexts they were chosen to be the major structuring element of this review of hyperspectral approaches; in each case a short introduction will describe their relevance to sustainable forest management.

3.3. Biophysical Parameter Retrieval Strategies

Absorption features in the near infrared region of the spectrum (1000-2500 nm) are a function of the bending and stretching vibrations of biochemical bonds (between, for example, hydrogen-carbon and nitrogen-oxygen atoms) together with their harmonics and overtones. In the visible region, chlorophyll and carotenoid pigments have strong absorption due to electron energy transitions (e.g. Dawson et al. 1998b). Different methods exist to retrieve leaf and canopy characteristics from reflectance measurements (e.g. Blackburn 2007; Kimes et al. 2000; Weiss and Baret 1999):

Empirical relationships (indices and/or multiple regressions): the principle is to combine several reflectances measured on narrow or large spectral bands into mathematical combinations and to correlate them to a particular characteristic of the observed surface. These relationships are calibrated based on an experimental or simulated reflectance database (built up on radiative transfer models). These methods are simple, but have some limits: when calibrated to an experimental database, the representativeness of the relationships is limited to the representativeness of the database (figure 1). Moreover, indices and multiple regressions may be sensitive to more than one single characteristic. They are also

sensitive to atmospheric conditions, view geometry, and spatial resolution, and therefore they must usually be calibrated for each image.

Model inversions: this method uses models that simulate reflectance spectra from leaf, canopy and soil characteristics and then attempts to derive leaf and canopy parameters by inverting the model. A typical numerical inversion protocol (e.g. Bicheron and Leroy 1999) consists of fixing some of the parameters to reasonable values and of determining the other parameters (free parameters) by minimizing a function of difference between observed (ρ_{meas}) and modeled (ρ_{mod}) reflectance. This function, called merit function, was chosen to be identical with that of Nilson and Kuusk (1989):

$$F = \sum_{i=1}^n \frac{(\rho_{\text{meas}}^i - \rho_{\text{mod}}^i)^2}{\rho_{\text{mean}}^i} + \sum_{i=1}^m [(x_i - x_{i,b})^2 w_i]$$

where n is the number of observations and m the number of free parameters. $x_{i,b}$ is the limiting value of parameter i , and $w_i=0$ if $x_{i,\text{min}} < x_i < x_{i,\text{max}}$ and $w_i=w$ otherwise, with w a very large given value. The extreme values of parameters correspond to their validity domain. An efficient minimization method is, for example, the optimized simplex method of Nelder and Mead (1965), which is the method recommended by Privette et al. (1994) after having tested several different inversion methods. As noted by (Bacour et al. 2006), inversion techniques based on pre-computed reflectance databases are often preferred to more computationally heavy iterative methods for operational applications. Among the computationally efficient methods often used are Look-Up Tables and Neural Networks (Bacour et al. 2006; Baret et al. 2007; Schlerf and Atzberger 2006).

Both methods are dependent on simulated or measured training databases. While uncertainties in measurements and models may result in large variation in results, numerical inversion strategies have to cope with other difficulties: inverse problems are concerned with determining causes for a desired or an observed effect or calibrating the parameters of a mathematical model to reproduce observations. Inverse problems most often do not fulfill important postulates of *well-posedness*: they might not have a solution in the strict sense, solutions might not be unique and/or might not depend continuously on the data. Inversion of such models often gives a large number of different possible solutions, i.e. they are ill-posed. Therefore, the use of efficient regularization strategies is of great importance for numerical inversion strategies.

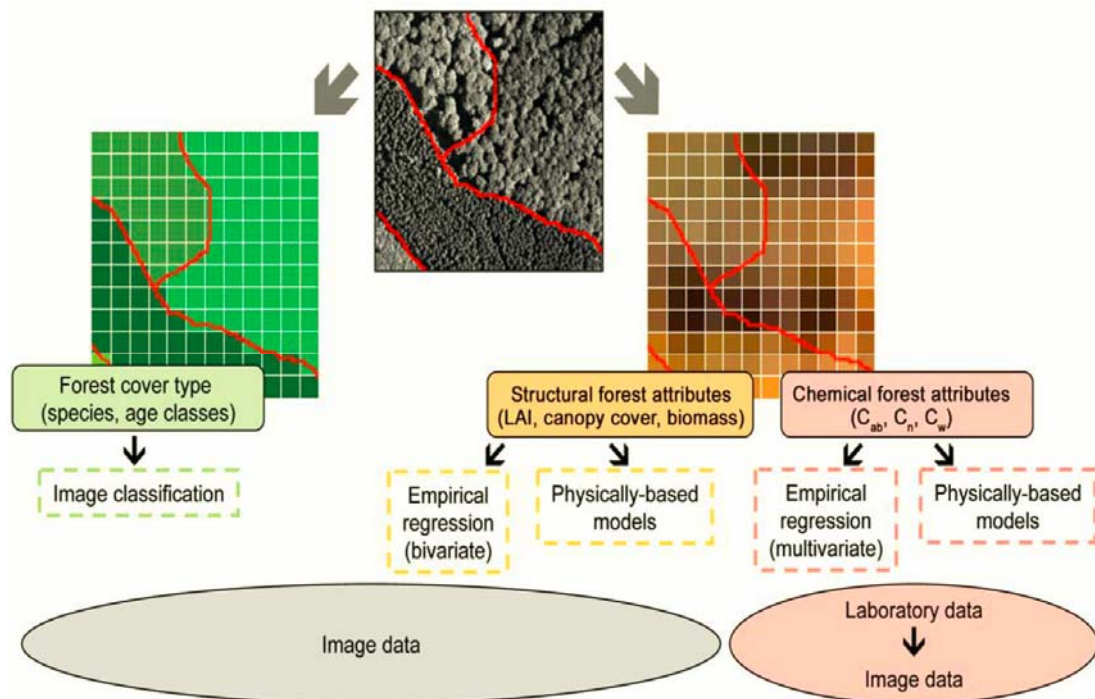


Figure : Strategies to extract forest attributes from remote sensing data as implemented within the framework of forest research (from Schlerf 2006).

3.3.1. Empirical Relationships

In the laboratory, leaf pigments are determined in solution by spectrophotometric analysis after extraction with organic solvents (Lichtenthaler 1987; Porra et al. 1989). Evidence from leaf and canopy experiments has indicated that narrow-band spectroscopy over the optical wavelengths is a promising approach for quantifying pigment concentrations. Because of this, high spectral resolution sensors on aircrafts or satellites (imaging spectrometers) were expected to be much more suitable for quantifying vegetation pigment concentrations (and other canopy parameters) than broad spectral band instruments (Verstraete et al. 1999). Pigment analysis with non-destructive optical methods (transmittance and reflectance spectroscopy) has meanwhile reached a high degree of maturity (Gamon and Surfus 1999; Gitelson and Merzlyak 1994a; Gitelson et al. 1996; Lichtenthaler et al. 1996; Markwell et al. 1995).

Unfortunately, these predictive equations proved to lack robustness and portability: they strongly depend on the study area and on the experimental conditions of the reflectance acquisition. In the transition from the controlled conditions of the laboratory to airborne studies, a number of perturbing effects are introduced, including variable solar illumination intensity and angle, both related to a specific biochemical of interest (water, viewing geometry, atmospheric conditions, vegetation canopy architecture [leaf area index (LAI) and canopy cover] and understory. Also, some caution is advised when using statistical approaches: a study of Grossman et al. (1996), for example, demonstrated that the bands selected by stepwise multiple linear regression for a given chemical (nitrogen, carbon, lignin, etc.) and a given spectral transformation ($\log(1/\square)$, first derivative, second derivative) did not correspond with bands selected in other studies, and band selection was very sensitive to the samples included in the dataset. These concerns led to the advancement of analytical

techniques for estimating foliar biochemical content from canopy reflectance spectra, such as radiative transfer modeling (Dawson et al. 1999).

3.3.2. Reflectance Models

Since the mid nineties, the broad use of leaf radiative transfer models such as PROSPECT (Jacquemoud and Baret 1990) for broadleaf species, LIBERTY (Dawson et al. 1998b) based on radiative transfer characterization in needles, and LEAFMOD (Ganapol et al. 1998) among others, enable the simulation of the leaf optical properties as a function of leaf structural and biochemical constituents.

Modeling Leaf or Needle Reflectance

The leaf reflectance model PROSPECT (Jacquemoud and Baret 1990; Jacquemoud et al. 1996) is a plate model which considers the leaf as a succession of absorbing layers. It calculates the leaf hemispherical reflectance and transmittance between 400 and 2500 nm, originally with a 5-nm step as a function of leaf structure index (N), leaf chlorophyll content (C_{ab} , $\mu\text{g}/\text{cm}^2$), leaf water content (C_w , g/cm^2), and leaf mass per area (C_m , g/m^2).

The reflectance is calculated using the specific absorption coefficients K of each component which depends on wavelength but not on species. The total absorption coefficient k for one layer is calculated with

$$k(\lambda) = k_a(\lambda) + \frac{C_{ab}}{N} K_{ab}(\lambda) + \frac{C_m}{N} K_m(\lambda) + \frac{C_w}{N} K_w(\lambda)$$

where λ is the wavelength, k_a the absorption of an “albino” leaf (taking into account the absorption by all other constituents than C_{ab} , C_w , and C_m before 500 nm), and K_{ab} , K_m , and K_w the specific absorption coefficients of chlorophyll a + b, dry matter, and water, respectively. They were originally obtained by inversion of the model on 63 leaves (LOPEX data set) with a step of 5 nm (Jacquemoud et al. 1996). Scattering is described by a spectral index of refraction and a parameter (N) describing the leaf mesophyll structure.

Since 1990 several versions of the model had been released which mainly introduced new biochemical constituents, mostly cell wall molecules such as cellulose, lignin and protein (e.g. Fourty et al. 1996; Jacquemoud et al. 1996). Although successfully used in many studies, the PROSPECT model was lately found to be not accurate enough to discriminate between the key pigments important for physiological and ecological applications and for evaluating certain spectral indices (Le Maire et al. 2004). After Le Maire et al (2004) had already extended the spectral resolution of the model from 5 to 1 nm, Feret et al. (2008) refined the core of the PROSPECT model by computing a new refractive index spectrum, by specifying a more realistic surface roughness parameter, and by developing an optimized calibration with regard to the specific absorption coefficients for water, dry matter and different pigments. The improved (1-nm resolution) and recalibrated version of PROSPECT calculates the leaf hemispherical reflectance and transmittance between 400 and 2500 nm as a function of leaf structure index (N), leaf chlorophyll content ($\mu\text{g}/\text{cm}^2$), leaf water content (g/cm^2), and leafmass per area (g/m^2). The resulting model versions PROSPECT-4 and PROSPECT-5 (no difference in the IR) are identical in retrieving water and dry matter concentrations; the difference is in the separation of total chlorophylls and total carotenoids, which improves the chlorophyll retrieval in PROSPECT-5. This slight improvement is due to a

better modeling of leaf optical properties, and is particularly significant for light-green leaves (Ferret et al. 2008).

SLOP (stochastic model for leaf optical properties) describes the radiative transfer of light within leaves as stochastic process based on the Markov chain theory (Maier et al. 1999). The crucial point in SLOP is to determine the transition probabilities. They are calculated with the aid of Beer's law from the optical parameters (i.e., the specific absorption coefficients of the different plant constituents and the scattering coefficients), the concentrations of the constituents, and the geometrical dimensions (i.e., thicknesses of the leaf layers and diameter of the chloroplasts).

LEAFMOD¹ (Ganapol et al. 1998) relies on the fact that, while light is moving in a complicated medium, natural averaging occurs in such way that the simpler assumption of isotropic scattering and uniform absorption seems to capture the transport effects (Morris et al. 2008). The model also has the ability to include chemistry as a key element to dominating the absorption process; different concentrations of chlorophyll, water, lignin and cellulose can be specified to model the optical properties of single leaves.

Leaf models have usually been based upon broadleaf vegetation where the leaf structure is considered to be an infinitely extending plane having distinct layers. Conifer needles, however, present their own particular problem. They do not contain a well-defined palisade layer, and so a transverse section of a pine needle will display roughly spherical cells. There are also problems of how to characterize and model the pine foliage elements. Because of the complex spatial distribution of pine canopies, it may be more appropriate to treat shoots (clumped needles) as the independently located foliage element instead of individual needles. Finally, their shape and size make it difficult to accurately measure the spectral properties of individual needles even in the laboratory. The LIBERTY (Leaf Incorporating Biochemistry Exhibiting Reflectance and Transmittance Yields) reflectance model (Dawson et al. 1998b) was developed specifically to address these problems.

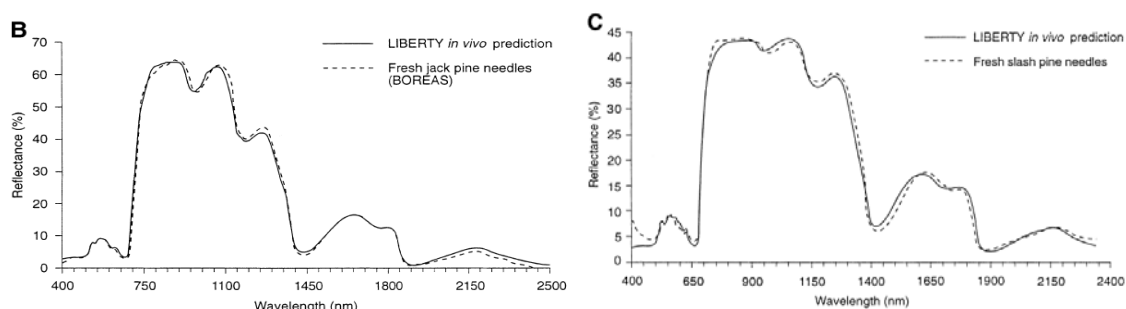


Figure 2: LIBERTY-predicted and measured Jack Pine (left) and Slash Pine needle reflectance spectra (from Dawson et al. 1998b).

The objective was to generically characterize and model conifer (particularly pine) needles at the cellular level by adapting Melamed's theory of light interaction with suspended powders (Melamed 1963) and infer leaf optical parameters from stacked needles in the laboratory.

¹ Leaf Experimental Absorptivity Feasibility MODEL

For pigment retrieval, wavelength corrected *in vitro* absorption data were incorporated into the LIBERTY model, the water absorption coefficient for LIBERTY was based upon the published absorption coefficients of pure distilled water over the spectral range 750–2500 nm (Curcio and Petty 1951), which has been shown to be in agreement with published absorption coefficients of *in vivo* leaf water (Jacquemoud and Baret 1990) estimated from PROSPECT inversion methods. The absorption coefficients of lignin and cellulose have similar features and their combined *in vivo* absorption peaks are difficult to separate due to their intimate mixture. Refractive indexes incorporated into LIBERTY were adopted from a regression equation of calculated refractive indexes (Jacquemoud and Baret 1990) against wavelength as a best approximation to the average refractive indices of wet mesophyll cells for the 400–2500 nm wavelength region, respectively (Dawson et al. 1998b).

LIBERTY has been validated against high quality laboratory measurements and provided excellent simulation results for dried and fresh needle (figure 2). An important difference to PROSPECT (with basically four simulation parameters, i.e. N, Cab, Cw, and Cm) is that the LIBERTY requires substantially more input parameters to run in the simulation mode (i.e. an average cell diameter, an intercellular air space descriptor, a leaf thickness parameter, a baseline and albino absorption parameter, and then the chlorophyll, water, lignin/cellulose and nitrogen contents). This might render numerical inversion strategies more complicated, unless part of these variables can be kept constant for a range of species.

Modeling Forest Canopy Reflectance

Both, PROSPECT and LIBERTY, can be coupled with a suitable canopy model for investigations of forest canopy reflectance. Initially, modeling studies were conducted with rather simple models (i.e., turbid-medium-based canopy models) (e.g. Jacquemoud 1993; Jacquemoud et al. 1995) which involved the coupling of the PROSPECT leaf optical properties model (Jacquemoud and Baret 1990) and the SAIL canopy reflectance model (Verhoef 1984)². Although more advanced strategies have been developed (e.g. Kötz et al. 2005; Verhoef and Bach 2007) a major limitation of the turbid medium models remains that they do not account for forest canopy architecture variables such as tree crown closure, tree density, tree heights, and shapes and dimensions of crowns, which may lead to incorrect estimation of forest reflectance (Gastellu-Etchegorry et al. 1999).

Over the past few years, research in this area has been extended to the full characterization of the radiative transfer within heterogeneous canopies such as deciduous and coniferous forests (Castellu-Etchegorry and Bruniqel-Pinel 2001; Dawson et al. 1999; Gastellu-Etchegorry and Bruniqel-Pinel 2001). Forest canopies are characterized by high horizontal and vertical heterogeneity; coniferous forest, in particular, exhibit a complex canopy structure which has to be considered at the needle and shoot levels, assessing the well-known clumping effect of needles, at the crown level, and at the forest stand level (e.g. Chen and Leblanc 1997). Consequently, the radiative transfer within a forest canopy depends on the spatial distribution of the canopy elements relative to each other and on the subsequent complex radiative processes such as multiple scattering, mutual shading of the crowns, and shading of the background.

² Jacquemoud et al. (2000) have compared the PROSPECT/SAIL canopy reflectance model with three different turbid media canopy reflectance models (each coupled to PROSPECT) with rather consistent results

In this case, three-dimensional canopy radiative transfer models (RTM) are required to parameterize the heterogeneous canopy structure appropriately (e.g. Atzberger 2000; Chen and Leblanc 1997; Disney et al. 2006; Govaerts and Verstraete 1998; Huemmrich 2001; Kuusk and Nilson 2000; North 1996; Schlerf and Atzberger 2006).

Unfortunately, the inverse solution of a RTM is not necessarily unique; the ill-posed nature of the RTM inversion increases with the complexity of the observed medium and the employed model (Combal et al. 2002). Ray-tracing, computer simulation or Markov chain models (Gastellu-Etchegorry et al. 1996; Govaerts and Verstraete 1998; Kuusk and Nilson 2000; North 1996), for example, compute the path of photons through the canopy to determine the direction of the incident rays and the direction of scattering. FLIGHT (North 1996), for example, is a three-dimensional ray-tracing model using Monte Carlo techniques for the radiative transfer within crown boundaries and deterministic ray tracing between the crowns and other canopy components. The canopy structure is represented by geometric primitives defined by the crown shape and size, tree height, position, and distribution. Contrary to GeoSAIL, the geometric representation of FLIGHT deals explicitly with crown overlapping, mutual shading, and multiple scattering between crowns. Each crown is assumed to be homogeneous, characterized by its structural variables as well as by its foliage optical properties. The characterization of the crown may vary for each tree. FLIGHT calculates directional reflectance by accumulating photons in predefined solid view angles. Due to the complex structure and the large number of input parameters required, these models are particularly difficult to invert (e.g. Goel 1988).

Therefore, simplified yet powerful alternatives have been proposed. Hybrid or geometric optics RTMs are combinations of geometrical and turbid medium models, i.e. the geometric shapes representing, for instance, tree crowns, are not considered as being opaque but are treated as a turbid medium. Usually, geometric optical models estimate the fraction of a scene that make up the reflectance components; these are in effect the sunlit and shadowed proportions of the canopy element (crown) and understory surfaces. The vegetation cover is treated as an assemblage of three-dimensional vegetation filled objects that are distinct from one another and are placed on a contrasting background.

The relatively simple radiative transfer model GeoSAIL (Huemmrich 2001) combines a simple geometric model (Jasinski 1996) with an adapted version of the SAIL model³ (Verhoef 1984) that provides the reflectance and transmittance of the tree crowns. The geometric sub-model determines the fraction of the illuminated and shadowed scene components as a function of canopy coverage, crown shape, and illumination angle; trees are assumed to be identical and to have no crown overlap, and the model does not account for mutual shading. Observation geometry is limited to nadir viewing. More advanced versions of this type of GORT approach are based on the Forest Light Interaction Model (FLIM) (Rosema et al. 1992) which has later been coupled to a linked PROSPECT/LIBERTY+SAILH⁴ model termed INFORM⁵ (Atzberger 2000; Schlerf and Atzberger 2006).

³ which can account for the contribution of multiple canopy components with different optical properties, leaf area index, and foliage inclination angles

⁴ SAILH considers the canopy hot spot effect

⁵ Invertible Forest Reflectance Model

3.3.3. Hybrid Approaches

An important limitation in defining suitable spectral indices for pigment retrieval ***based on experimentally collected data*** results from the fact that the samples do not necessarily cover the “full” dynamic range of variables and include experimental noise in relation to specific environmental conditions. Establishing a truly comprehensive measurement data base might be feasible at the leaf scale (e.g. Hosgood et al. 1995) but is not conceivable at the level of forest canopies (Le Maire et al. 2008). Therefore, efforts have been made to create large synthetic databases containing leaf reflectance spectra and their corresponding canopy characteristics from reflectance models to test and evaluate pigment-sensitive spectral indices, sometimes in combination between modeled and experimental data (Blackburn and Ferwerda 2008; Broge and Leblanc 2000; Le Maire et al. 2004; Le Maire et al. 2008). Broge & Leblanc (2000) used a database of vegetation canopy spectra generated with a coupled PROSPECT/SAIL model to analyse different spectral indices with regard to their ability to derive ***canopy chlorophyll concentrations***. Beside classical broadband vegetation indices (not considered here) they tested a few multi-band and hyperspectral indices related to the red edge feature. Le Maire et al. (2004) used the PROSPECT leaf reflectance model (Jacquemoud and Baret 1990) to develop, test, and compare several leaf chlorophyll indices for identifying “universal” chlorophyll (a + b) indices which would be applicable to a wide range of species and leaf structure.

Such a database has many advantages: a large variety of canopy characteristics are represented (thousands of spectra); the influence of each characteristic can be totally decoupled from that of others; and the effect of a particular characteristic on the spectra is based on physical processes that are modeled at a small scale. Therefore, well established indices obtained on such a large simulated database may potentially be applied to a wide range of spectra. However, the use of a model relies on its capacity to correctly simulate the reflectance of a wide range of canopies. Thus, it is essential to test these indices on experimental measurements (Le Maire et al. 2004).

3.4. Foliar Biochemistry on Leaf and Canopy Level

Ecosystems play an important role in the exchange of water, energy and greenhouse gases between soil, vegetation, and the atmosphere. The ability to detect changes in ecosystem processes such as carbon fixation, nutrient cycling, net primary production, and litter decomposition is an important part in defining global biogeochemical cycles and identifying changes in climate. In models of forest ecosystems, these processes have been linked to canopy biochemical content, specifically to nitrogen, lignin, and cellulose concentrations.

Knowledge of pigments present in plant leaves is therefore an important prerequisite for improved assessment and quantification of vegetation physiology and vitality. Since estimates of canopy chemistry by traditional field sampling methods are time-consuming and difficult to make for large regional and global studies, the remote sensing of foliar biochemistry (nutrients, pigments) as an indicator of stress phenomena or pests, plant diseases and other calamities has long been of interest to forest managers and ecologists.

Three types of pigments determine leaf color as the result of selective light absorption: chlorophylls (two major types in higher plants, chlorophyll a and chlorophyll b), carotenoids (including β -carotene and xanthophylls), and anthocyanins. Pigment content and composition are related to the leaf physiological status and are present in variable portions during the differentiation and aging of leaves. Some situations can block their production. For example, nutrient deficiency and the effect of abiotic stress – such as ozone or sulfur dioxide air pollution, heavy metals, viral attack or water deficiency – can cause changes in the optical properties of vegetation. While chlorophyll concentrations provide an indication of photosynthetic functioning and potential maximum CO₂ assimilation rates, carotenoids contribute to light-harvesting, but also play a photo-protective role and indicate down-regulation of photosynthesis (Feret et al. 2008; Gamon et al. 1992). Nitrogen and lignin are related respectively to carbon allocation (Schimel 1995) and the rate of nutrient cycling via their influence on decomposition rates (Meentemeyer 1978). Chlorophyll concentration is also highly correlated to nitrogen, and it has therefore become a key parameter for studying plant canopies (Gitelson et al. 2003; Le Maire et al. 2008).

There are many examples where data acquired by imaging spectrometers have been related to foliar biochemical properties (e.g. Gastellu-Etchegorry et al. 1995; Wessman 1994). Earlier studies have mostly used stepwise regression to develop predictive relationships between remotely sensed data recorded in narrow spectral wavebands and the biochemical variable of interest (e.g., cellulose, chlorophyll, lignin, nitrogen and starch). However, stepwise regression is open to criticism (Curran 1989) and alternative techniques have been proposed, including the estimate of biochemical variables via reflectance models.

In the transition from the leaf to the canopy level, strong disturbing effects are introduced, such as canopy architecture (leaf area index, leaf angle distribution) and influence of soil background. Compared to controlled laboratory conditions, airborne or spaceborne data are affected by further disturbances, such as variable solar illumination and atmospheric conditions, along with instrument characteristics (signal-to-noise ratio, spectral bandwidth, geometric field of view). Together, these factors cause a number of problems in the usage of remote sensing data to the determination of foliar biochemistry. Despite these problems several studies (Peterson et al., 1988; Wessman et al., 1988, 1994a; Johnson et al., 1994; Gastellu-Etchegorry et al., 1995) have suggested that spectroradiometric measurements of plant canopies can be correlated with variations in canopy chemistry, involving lignin, nitrogen and cellulose concentrations.

3.4.1. Pigment Concentration

Several types of empirical and model-based approaches have been tested and identified as being of values in predicting pigment concentrations from spectral reflectance measurements. The following general findings can be summarized (Blackburn 2002):

Reflectance measurements in various individual narrow bands have provided evidence that at wavelengths where the absorption coefficients of pigments are high, reflectance is more sensitive to low concentrations, while spectral regions with low absorption are more sensitive to higher pigment concentrations (Jacquemoud and Baret 1990).

The use of ratios of reflectance in narrow bands has been proposed as a method of solving the problems of the overlapping absorption spectra of different pigments and the effects of leaf structure, leaf surface interactions and canopy structure. Most authors used ratios of bands from the visible and near infrared, some identify only visible wavelengths and others use narrow wavebands in the region of the red edge (e.g. Blackburn 1998).

The characteristics of the first and second derivatives of reflectance spectra have been suggested as superior to spectral reflectance itself, mainly because of their ability to reduce variability due to changes in illumination or background reflectance. Most popular is the use of derivatives to define the wavelength position of the red edge (λ_{RE}), which has shown to be sensitive to total chlorophyll (e.g. Gitelson et al. 1996)

In the following section, we shall review some of the proposed indices in more detail, where the following categories of spectral indices are considered, where major emphasis will be placed on their applicability to forest tree species:

Indices using a single reflectance or a difference between two wavelengths

Simple Ratio of reflectance (SR)

Normalized ratios of differences of reflectance (ND)

Indices using reflectance derivatives⁶

The most recent literature references to this topic is the work of Le Maire et al. (2004; 2008) and Blackburn (2007). It should also be acknowledged that classical broadband indices will not be considered in detail in this state-of-the-art review.

3.4.2. Chlorophyll: Ratio and Difference Indices

One of the most recent and thorough studies on **chlorophyll-sensitive indices** (Le Maire et al. 2004) used leaf samples from different broad leaf tree species (*Acer pseudoplatanus*, *Betula* sp., *Fagus sylvatica*, *Fraxinus excelsior*, *Prunus avium*, *Quercus robur*, *Quercus ilex*, *Salix* sp.) in combination with a leaf reflectance database simulated with PROSPECT (Jacquemoud and Baret 1990), and applied all leaf chlorophyll indices published from 1973 to 2002. The authors demonstrated that modified Simple Ratios and modified Normalized Differences still are optimum indices. Among these one finds the mSR and mND indices of Sims & Gamon (2002), i.e.

$$mSR = (\rho_{ref} - \rho_{445}) / (\rho_{idx} - \rho_{445})$$

and

$$mND = (\rho_{ref} - \rho_{idx}) / (\rho_{ref} + \rho_{idx} - 2\rho_{445})$$

with $\lambda_{ref} = 750$ and $\lambda_{idx} = 705$ nm; based on their optimization procedure, Le Maire et al. (2004) suggest alternative “base” wavelengths (i.e. 434 instead of 445 nm). Also among the best indices is the index

$$(\rho_{750} - \rho_{705}) / (\rho_{750} + \rho_{705})$$

of Gitelson and Merzlyak (1994b). Relatively low chlorophyll contents are sufficient to saturate absorption in the 660–680 nm region and thus reduce the sensitivity of this wavelength region to high chlorophyll contents. Consequently, empirical models for

⁶ precise derivatives can only be obtained with hyperspectral data

prediction of chlorophyll content from reflectance should be based on reflectance in the 550 or 700 nm regions where higher chlorophyll contents are required to saturate the absorbance.

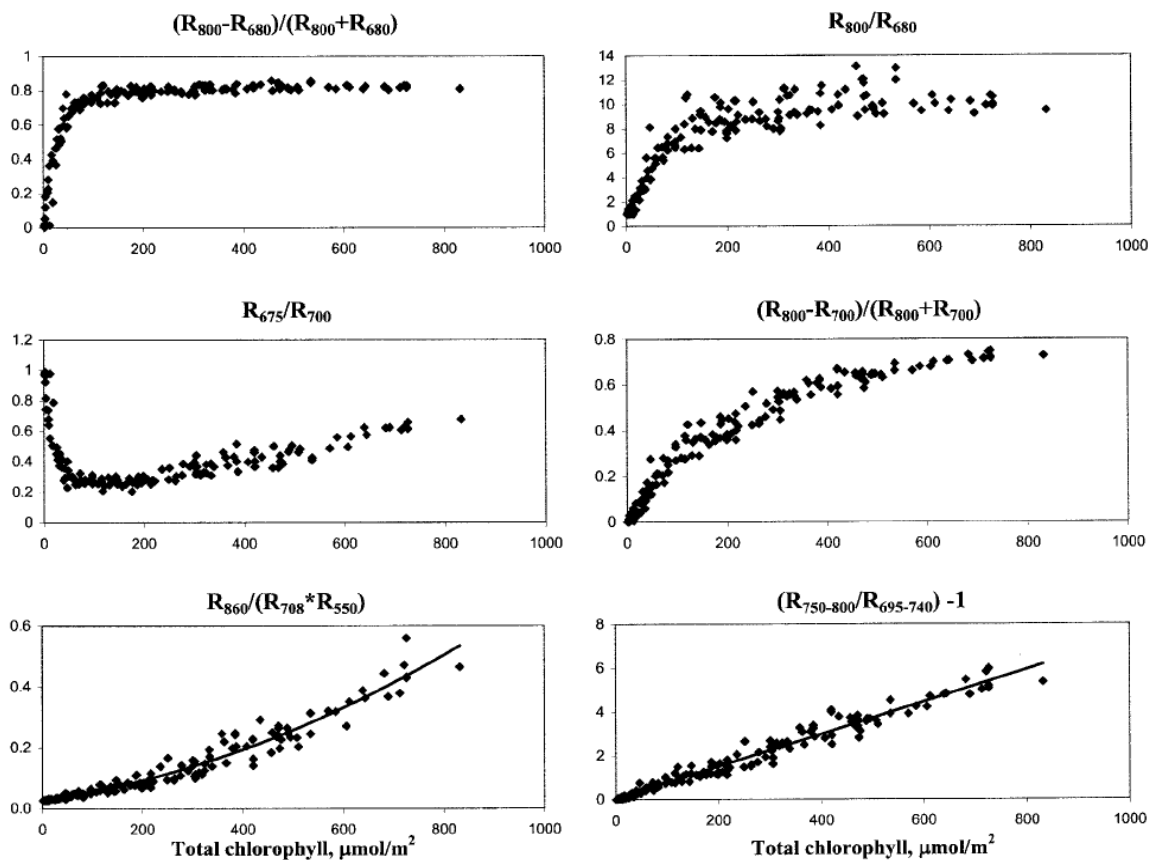


Figure 3: Scatter plots indicating the relationship between various reflectance indices and total Chl content (from Gitelson et al. 2003).

Gitelson and Merzlyak (1994a) had been among the first to prove that reflectance in the spectral bands located quite far from the main pigment absorption bands, such as

$$\frac{(\rho_{750} - \rho_{700})}{(\rho_{750} + \rho_{700})},$$

were closely related to chlorophyll content (with somewhat reduced sensitivity to chlorophyll concentrations above 400 $\mu\text{mol m}^{-2}$). Sims and Gamon (2002) in fact confirmed these results but showed that the correlation was weaker when **applied across a wide range of plant species**.

With a focus on several tree species (beech, maple, chestnut) Gitelson et al. (2003) later developed a range of reciprocal reflectance indices of the form

$$\rho_A^{-1},$$

$$(\rho_A^{-1} - \rho_{NIR}^{-1}),$$

and, by using the product of the previous index and ρ_{NIR} , suggested

$$(\rho_{NIR}/\rho_A) - 1,$$

as an optimized chlorophyll index (figure 3) which is not yet included in the study of Le Maire et al. (2004). These indices are a) linearly proportional to chlorophyll with intercepts close to zero, b) extend the spectral ranges of the reference bands (525-555 and 695-735 nm), and c) are also sensitive to very low concentrations (total range 14-670 $\mu\text{mol m}^{-2}$).

The increased sensitivity of the selected wavelength ranges (green and red edges) is obviously due to the increased light penetration into the leaf tissue (Gitelson et al. 2003). When applying alternative indices proposed by Blackburn (1998), Chappelle et al. (1992) and Datt (1998) to the same data, problems of reduced sensitivity to either low or high pigment concentration or inconsistent behavior with low values became apparent. Gitelson et al. (2003) recommend wavebands at 550 ± 20 nm, 715 ± 20 nm, and 450 ± 20 nm with the NIR band above 750 nm for estimating chlorophyll; for anthocyanin-containing leaves, spectral bands 715 ± 20 nm, 450 ± 20 nm and a NIR band above 750 nm are recommended. Quite importantly with regard to hyperspectral imaging systems, the use of **relative large bandpasses allows for a significant increase in sensitivity and signal-to-noise-ratio**.

Pigment-related indices which involve wavelengths close to or within the absorption maxima of chlorophylls perform clearly worse. Blackburn (1998), for example, tested several pigment-related ratio indices for retrieving chlorophyll a and b as well as carotenoid concentrations in bracken leaves (and canopies from) narrow-band reflectance (ρ). The used wavebands (in nm) were selected with regard to primary absorption wings of the selected substances:

$$\rho_{800}/\rho_{680}, \rho_{800}/\rho_{635}, \text{ and } \rho_{800}/\rho_{470}.$$

The derived regression models of the form $y = ax^b$ (where x is the corresponding “base” value) had coefficients of determination between 0.96 and 0.94, and thereby exceeded the performance of several normalized difference and 1st/2nd order derivative indices tested by the same author (Blackburn 1998), but were sensitive to saturation in lower and higher concentration ranges due to the strong non-linearity of the relationships. And, not to forget, bracken canopies represent very special cases of homogeneous turbid media, and the results on canopy level are certainly not representative for forest canopies.

In addition to testing the range of indices described earlier, Le Maire et al. (2004) also tried to optimize the best wavelengths for suitable indices and defined a new type of index, the Double Difference (DD) index:

$$DD = \int_b^{b+\Delta} \rho' d\lambda - \int_a^{a+\Delta} \rho' d\lambda -$$

This index is the difference of the integral of reflectance derivatives, where a and b are two different wavelengths, and Δ is the integration window. Preliminary studies suggest that a and b are near 670 and 720 nm, and Δ is approximately 30 nm (Le Maire et al. 2004). This index was chosen because it represents the changes in the first derivative in the red-edge region when chlorophyll varies which is linked to the so-called “peak jump” feature (see following chapter). A simple integration gives the effective formulation of the Double Difference index (DD):

$$DD = (\rho_{b+\Delta} - \rho_b) - (\rho_{a+\Delta} - \rho_a)$$

This type of index has the advantage to be computationally simple and to keep the characteristics of hyperspectral indices based on second derivatives. The constant and linear terms in reflectance are actually removed (because of the double difference with the same Δ

value). This property should be more interesting at the canopy level where soil spectrum shows linear behavior in the visible domain and where constant values may come from a bias in sensor or atmospheric effects. Le Maire et al. (2004) obtained the best results with wavelengths 672 and 720 nm and a Δ of 29 nm, i.e.

$$DD = (\rho_{749} - \rho_{720}) - (\rho_{701} - \rho_{672}).$$

The Double Difference Index had the best performance on the combined experimental and modeled database. A simple modified difference ratio mSR (Datt 1999) gave the best results among all examined published indices (until 2002) on the experimental database.

Some caution might still be required with the results of Le Maire et al. (2004) because there were indications that the PROSPECT model needed more careful calibration with respect to absorption coefficients and refractive index. But, since indices for **chlorophyll estimation** have been tested by several authors across a wide range of species and leaf structures there is reason to believe **that these indices could be applied across species without extensive calibration for each species**.

Estimation of leaf **carotenoid content** from reflectance is much more difficult than estimation of chlorophyll because of the overlap between the chlorophyll and carotenoid absorption peaks and because of the higher concentration of chlorophyll than carotenoid in most leaves. Therefore reflectance indices have proved more successful for the estimation of the ratio of carotenoid to chlorophyll, than in the estimation of the absolute carotenoid content (Merzlyak et al. 1999; Penuelas et al. 1995). Attempts have been made to estimate total carotenoids from reflectance (Chappelle et al. 1992; Datt 1998) but these indices have not shown good generality when applied to other datasets. Most indices for estimation of carotenoid/chlorophyll ratios are based on the comparison of reflectance in the region of the carotenoid absorption peak (400–500 nm) with reflectance in the red region, which is influenced only by chlorophyll.

Sims & Gamon (2002) tested several indices, among which the “photochemical reflectance index” (PRI) has special importance because significant relationships with light-use-efficiency (LUE), an important state variable in production models, have been identified (Gamon et al. 1992; Gamon et al. 1997; Sims et al. 2006). The PRI (see also Gamon et al. 1992) is defined by

$$PRI = \frac{(\rho_{681} - \rho_{670})}{(\rho_{681} + \rho_{670})}$$

and thus measures the relative reflectance on either side of the green peak (550 nm), one side being affected only by chlorophyll absorbance and the other by chlorophyll + carotenoid absorbance. For retrieving chlorophylls Sims and Gamon (2002) proposed a modified normalized difference index

$$mND705 = \frac{(\rho_{750} - \rho_{705})}{(\rho_{750} + \rho_{705} - 2\rho_{445})}$$

and a modified simple ratio index

$$mSR705 = \frac{(\rho_{750} - \rho_{445})}{(\rho_{705} - \rho_{445})}$$

which both exhibited acceptable relationships to the total chlorophyll of a wide range of leaf samples.

3.4.3. Carotenoids and Anthocyanin

While many models relating Chl content to reflectance are quite robust in Chl prediction, only few models support anthocyanin and carotenoids content retrieval. Usually, reflectance indices have proved more successful for the estimation of the **ratio** of carotenoid to chlorophyll, than in the estimation of the absolute carotenoid content. In fact, the PRI (see previous section) exhibits a (weak) linear relationship with the chlorophyll to carotenoid ratio (Sims and Gamon 2002).

However, once more based on the principle that sensitive spectral indices involve a first spectral band (λ_1) that is maximally sensitive to absorption by the pigment of interest, a second band λ_2 where absorption by the pigment of interest is much lower than at λ_1 , and absorption by other pigments and the effect of backscattering are quite close to that at λ_1 , and a third spectral band λ_3 should be used where backscattering controls reflectance, Gitelson et al. (2006) proposed reciprocal reflectance indices of the form

$$[\rho_{\lambda_1}^{-1} - \rho_{\lambda_2}^{-1}] \cdot \rho_{\lambda_3}$$

For retrieving chlorophyll a, for example, it was recommended to use the NIR reflectance at 760 nm for ρ_{λ_3} and the green spectral range, yielding linear relationships between

$$\text{Chl} \text{ and } [\rho_{540-560}^{-1} - \rho_{\text{NIR}}^{-1}] \cdot \rho_{\text{NIR}}$$

which can be simplified to $(\rho_{\text{green}}/\rho_{\text{NIR}}) - 1$ (see also Gitelson et al. 2003). For retrieving

carotenoids, the authors proposed to relate

$$\text{Car}_{\text{green}} \text{ to } [\rho_{510-520}^{-1} - \rho_{560-570}^{-1}] \cdot \rho_{\text{NIR}}$$

$$\text{and Car}_{\text{rededge}} \text{ to } [\rho_{510-520}^{-1} - \rho_{650-710}^{-1}] \cdot \rho_{\text{NIR}}$$

and for retrieving anthocyanin to relate

$$\text{Anth to } [\rho_{530-570}^{-1} - \rho_{650-710}^{-1}] \cdot \rho_{\text{NIR}}$$

It is important to note that Blackburn and Ferwerda (2008) confirm the efficiency of this type of indices for retrieving chlorophyll concentrations on leaf level in a more recent study.

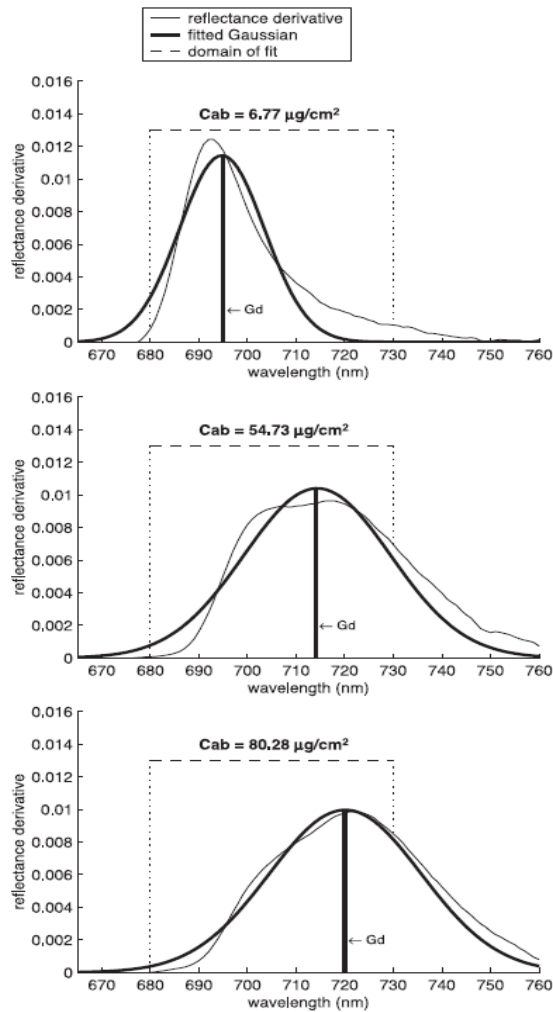


Figure 4: Three experimental reflectance derivative spectra with different chlorophyll contents. The Gd index is the centre of the Gaussian curve (providing an estimate of the REIP). Dashed lines show the chosen domain of fit (from Le Maire et al. 2004)

3.4.4. Red-Edge Position and Spectrum Derivatives

The red edge inflection point (REIP), which is the point of maximum slope, occurs between 680 and 750nm and provides a spectral measurement that is less sensitive to the effects of variable irradiance and background.

The increase in vegetative chlorophyll-a concentration during the growth cycle has been shown to cause a red-shift of the inflection point (λ_{RE}). It is argued that this phenomenon is caused by polymer forms of chlorophyll adding closely spaced absorption bands to the far red shoulder of the main chlorophyll-a band (e.g. Collins 1978). At the onset of senescence, the mesophyll structures in the plant tissue (effective near infrared reflectors) begin to collapse. Meanwhile, leaf chlorophyll decreases causing red reflectance to increase. These combined effects cause a blue-shift of the so-called “red-edge-inflection-point” (REIP).

The REIP can be determined with different methods. Miller et al. (1990) used an inverted Gaussian model to describe the variation of reflectance as a function of wavelength. This approach has the advantage that it has a built-in smoothing of the red edge spectral reflectance and has been used by several authors (e.g. Bonham-Carter 1988). The inverted Gaussian model is described with

$$\rho_\lambda = \rho_\infty - (\rho_\infty - \rho_0) \exp\left(-\frac{(\lambda - \lambda_0)^2}{2\sigma^2}\right)$$

where ρ_s is the “shoulder” reflectance at the NIR plateau (usually 780 – 800 nm); ρ_0 is the minimum reflectance in the chlorophyll absorption at 670 nm, σ the Gaussian shape parameter, such that the inflection point (REIP)⁷ is equal to $\rho_0 + \sigma$ (e.g. Bonham-Carter 1988). Le Maire et al. (2004) proposed a new technique which consists of fitting one Gaussian on the reflectance derivative in the red-edge region. The value of the index (Gd) is the centre (maximum) of the Gaussian (an estimation of the real REIP) (figure 4).

Another way of obtaining REIP is fitting a higher order polynomial to the reflectance data in the red edge spectral range (Broge and Leblanc 2000); a high-order polynomial will capture potential asymmetry of the red edge, whereas the inverted Gaussian model will average out such asymmetry. Dawson and Curran (1998) proposed a new way to determine REIP. They applied a technique known as Lagrangian interpolation, which is applied to the first-derivative transformation of the reflectance spectrum. The technique fits a second-order polynomial curve to three bands, from which the REIP is determined.

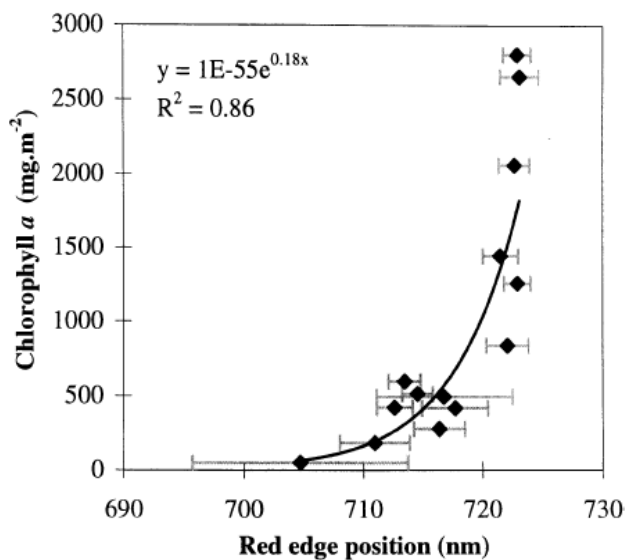


Figure 5: Relationship between the wavelength position of the reflectance red edge and the canopy concentration per unit area of Chl a (from Blackburn 1998)

Blackburn (1998) used the first derivative to identify the REIP (figure 5). The position of the red edge, ρ_{RE} had reasonably strong exponential relationships with the canopy concentration per unit area of chlorophyll a, b and carotenoids but much weaker correlations with pigment concentration per unit mass at the canopy and leaf scales. The first derivative (dR) of reflectance showed even stronger relationships with canopy pigment concentration per unit area, and dR at three specific wavelengths proved to be reasonably well correlated with pigment concentrations per unit mass at both leaf and canopy scales. Although high coefficients of determination are achieved, it is seen that the type of relationship is sensitive to saturation effects in low and high concentration ranges.

As already noted in earlier studies, a peak jump on the reflectance derivative (i.e. several local maxima) in the red-edge area was observed in experimental and modeled data for concentrations exceeding $45 \mu\text{g cm}^{-2}$. They could be explained by the characteristics of two associated chlorophyll absorption peaks (Le Maire et al. 2004). Therefore, **on the leaf level**, REIP-like indices and similar derivative-based indices showed bad performance and gave

⁷ the Gaussian function is fitted to the measured reflectance by adjusting the values of ρ_s , ρ_0 , λ_0 and σ

worse results than simpler properly chosen indices. With regard to the fact, that relationships between REIP and chlorophyll concentrations are non-linear (Blackburn 1998), their relative complexity does not appear justify their use in comparison to more accurate and simpler chlorophyll indices, a finding which is still to be confirmed for measurements on canopy level.

A classical empirical approach for estimating foliar chemistry is to establish an empirical model between the selected derivative features and the concentration of the desired leaf constituents. The efficiency of this approach obviously depends on the statistical algorithm applied. Smith et al. (2002), for example, converted reflectance values (r) to absorbance (a) using the equation $a = \log_{10}(1/r)$ and then applied a derivative transformation. The derivative spectrum provides a measure of the slope of the reflectance curve at every point and results in a spectrum in which baseline offsets (caused, for example, by varying sun-earth-sensor geometry and, to some extent, canopy background effects) have been removed or substantially minimized. In the following step, the most significant wavelengths are selected (e.g. Hruschka 1987). Relationships between spectra and chlorophyll (or nitrogen, by exploiting intercorrelation effects to chlorophyll) have for example been examined using partial least squares (PLS) regression, in which the full reflectance spectrum is collapsed into a smaller set of independent variables, or factors, with the measured data used directly during the spectral decomposition process (Kramer 1998; Udelhoven et al. 2003).

3.4.5. Alternative Pigment Estimation Strategies: Wavelet Analysis

Also Blackburn and Ferwerda (2008) employed leaf-scale radiative transfer models to generate very large spectral data sets which they used to develop and rigorously test refinements to an alternative estimation approach (wavelets) and compare it with existing spectral indices. Wavelets are mathematical functions that decompose a complex signal into different frequency components and each component is characterized with a resolution appropriate to its scale. This kind of approximation using superposition of functions is derived from Fourier analysis. However, wavelet analysis represents local spectral features as it can decompose into components localized in both time and frequency domains, while Fourier analysis can only represent frequency information. For Fourier analysis the new domain contains basis functions that are sines and cosines, while the new domain in wavelet analysis contains an infinite set of possible basis functions called wavelets, mother wavelets or analyzing wavelets.

When applied to reflectance spectra, an empirical model can be established between the wavelet coefficients that are assigned to the component sub-signals and the concentration of the desired leaf constituents. Blackburn & Ferwerda (2008) used 75 % of their data for constructing predictive stepwise regression models which were applied to the wavelet coefficients derived from both, reflectance and derivative spectra; 25 % of the data were used for testing. The results demonstrated that by decomposing leaf spectra by means of wavelets, the resultant coefficients can be used to generate accurate predictions of chlorophyll concentration, despite wide variations in the range of other biochemical and biophysical factors that influence leaf reflectance. Integrating the spectral response over multiple bands, i.e. exploiting particular scales of spectral variability (discussed below) was more important than the choice of wavelet function used to perform the transformation. In this experiment, derivative spectra appeared to be more suitable as input to wavelet analysis

than reflectance spectra, probably because derivative spectra consist of a series of peaks and troughs which oscillate around zero and thereby resemble a series of wavelet functions.

Since it has also been suggested that the use of spectral derivatives can reduce the influences upon canopy spectra of variations in illumination and soil/litter reflectance (Elvidge and Chen 1995) the approach might offer further benefits when applying wavelet analysis to canopy-scale data acquired by airborne or space-borne imaging spectrometers. The authors also compared the performance of the wavelet analysis with spectral indices that have been identified as efficient indicators in the previous section of this report.

Coefficients of determination and RMSE values indicated that the wavelet approach outperformed other indices, with the Double Difference index of Le Maire et al. (2008) and the chlorophyll indices of Gitelson et al. (2006) following next (see sections before); the modified difference and ratio indices of Sims and Gamon (2002) appeared less efficient.

The wavelet approach has reasonable implementation perspectives since appropriate tools to aid wavelet construction are available, for example in the MATLAB wavelet toolbox.

3.4.6. Additional Biochemical Constituents

Plant materials are composed largely of hydrogen, carbon, oxygen, and nitrogen. Thus, the absorption bands observed in reflectance spectra of vegetation arise from vibrations of C—O, O—H, C—H, and N—H bonds, as well as overtones, and combinations of these vibrations (Curran 1989). The absorptions from the different plant materials are similar and overlapping, so a single absorption band cannot be isolated and directly related to chemical abundance of one plant constituent.

Although stepwise multiple regression is meanwhile replaced by more efficient algorithms, such as for example Partial Least Squares Regression (PLSR) (e.g. Otto 1998; Wold et al. 2001) or Support Vector Machine Regression (SVM-R) (Burges 1998; Vapnik 1995) the basic problem is to select optimal spectral variables for representing the desired constituents. Kokaly and Clark (1999) proposed an approach where continuum removal (Clark and Roush 1984) was applied to broad absorption features in dry leaf spectra and absorption-band depths relative to the continuum were calculated. Band depths in each absorption feature were normalized using the depth at the center of the feature and also the area under the band depth curve. It is suggested that spectral changes due to nonfoliar influences are reduced by using continuum removal and normalization to the area of the absorption band (Kokaly and Clark 1999).

Several studies have suggested that empirical estimates based on remote spectroscopic measurements may be possible (e.g. Martin and Aber 1997). These studies used stepwise multiple linear regression to predict canopy chemistry from derivative reflectance spectra. This technology was adopted from a strategy developed about 40 years ago in the agriculture industry for the rapid estimation of forage quality from the reflectance spectra of dried and ground foliage (Norris et al. 1976). Strong relationships between the concentration of foliar chemicals and reflectance were also found by other researchers for dry and ground leaves using multiple regression techniques (e.g. Card et al. 1988). More reliable results

were obtained when normalized band depths were used in stepwise regression approaches instead of reflectance values (Curran et al. 2001; Kokaly and Clark 1999).

To bridge the gap between established laboratory methods and remote sensing, controlled experiments on fresh whole leaves have been undertaken by various researchers. However, the influence of water is strong throughout the near infrared region (1000-2500 nm) where most of the biochemicals have their absorption features. Consequently, leaf water can obscure absorption features related to foliar chemicals, such as protein, lignin, and cellulose in green leaf materials with considerable consequences for their estimation from reflectance spectra. For instance, Kokaly & Clark (1999) concluded that their method and those using $\log(1/\square)$ derivatives would be sensitive to variations in leaf reflectance that may be solely caused by changes in leaf water content.

Although the analysis of dried and ground leaves indicate that accurate prediction of chemical concentrations can be made, additional complexities at the remote sensing scale will be encountered, including: different instrument characteristics (S/N and bandpass), atmospheric effects, leaf water, fractional canopy coverage (e.g., the influence of soil background), and canopy architecture (e.g., leaf area index and leaf angle distribution). In fact, when correlating plant canopy chemistry to imaging spectrometer data the results at leaf and canopy scales were inconsistent, the derived regression equations were not reliable predictors for other remotely sensed data (Johnson et al. 1994; Martin and Aber 1997), and the use of regression techniques with derivative reflectance spectra were found to give inconsistent results between different forest sites (Grossman et al. 1996). The bands selected in their study lacked correspondence to those reported in other studies.

One important limiting factor to reliably estimate foliar chemicals is the signal-to-noise ratio of imaging spectrometry data. Of all the applications of imaging spectroscopy in recent years, the estimation of foliar chemical concentration has proved to be one of the most demanding in terms of signal-to-noise ratio (Peterson and Hubbard 1992). Specifications given in the literature on required SNRs for chemical estimates vary considerably. Gholz et al. (1996) compared minimum SNRs from a laboratory study (Nitrogen 37:1, Cellulose 65:1) with the approximate SNRs at vegetation reflectance given by the Jet Propulsion Laboratory and assessed data provided by the AVIRIS sensor to be sufficient for the estimation of foliar chemical concentrations. The minimum required SNR for this purpose has also been estimated by Smith and Curran (1996). From modeling the SNR, they showed that the required SNRs at nitrogen absorption features were always the smallest due to close relationships of spectral reflectance to protein and nitrogen concentrations. They suggest that out of three chemicals studied (nitrogen, lignin and cellulose) nitrogen could be estimated most successfully with remotely sensed data.

3.4.7. Estimating Leaf Biochemical Constituents with Reflectance Models

Estimation of chlorophyll from remotely sensed imagery can generally be achieved more reliably than the other chemicals, as the prominent chlorophyll absorption feature is not masked by leaf water. Jacquemoud et al. (1996) have used the LOPEX93 (Leaf Optical Properties Experiment) data set described in detail in (Hosgood et al. 1995) to validate the performance of the PROSPECT leaf reflectance model. It consists of about 120 leaf samples

representing woody and herbaceous species that were obtained from trees and crops near the Joint Research Centre in Ispra, Italy. A wide range of variation in leaf internal structure, pigments, water, and biochemistry contents was available, leading to a correspondingly wide range of variation in leaf optical properties. Chlorophyll was retrieved with reasonably high r^2 -values (0.68), while carbon based compounds with r^2 -values from 0.50 to 0.88; estimation of protein is still at issue (Jacquemoud et al. 1996). This study provided the starting point for applying PROSPECT in more studies. In fact, various authors have used reflectance models to successfully estimate chlorophyll from leaf or needle reflectance spectra (figure 6).

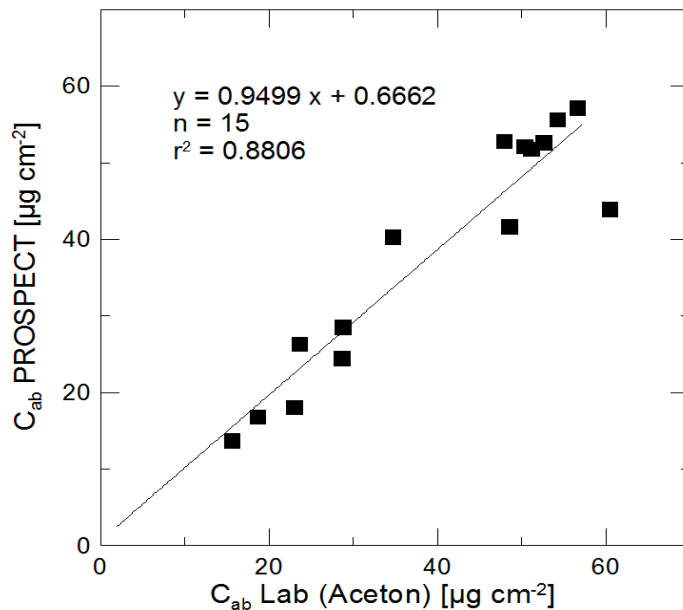


Figure 6: Relationship between laboratory measurements (Aceton extracts) of total chlorophyll concentration and the corresponding estimates from spectral measurements. These were obtained by numerical inversion of the PROSPECT model (version 3.01) for Beech (*Fagus Sylvatica*) leaves, where the wavelength range from 450 to 1000 nm was used (own experimental results, © Abt. Fernerkundung & Geobotanik, Universität Trier)

However, the inversion of a leaf reflectance model (PROSPECT) for other biochemicals than chlorophyll showed results of varying success. While Jacquemoud et al. (1996) obtained reasonable estimates on dry (but not on fresh) leaves, Fourty et al. (1996) were not able to retrieve any of the single biochemical compounds within dry leaves; total amount of dry matter per unit leaf area was the only variable to be accurately estimated. Fourty and Baret (1998) showed that the detailed biochemistry (protein, lignin, cellulose) was not accessible in an accurate way when observing a large range of species; they recommended working on a limited set of species, a common strategy for many more biophysical variable retrieval strategies.

3.4.8. Scaling Up: Leaf Biochemistry at Canopy Level

The extent to which **leaf chlorophyll concentration can be estimated from reflectance measurements at canopy and landscape scales** remains uncertain. Correlations between spectral indices and leaf chlorophyll have been demonstrated for uniform canopies (Blackburn 1998). However, most chlorophyll indices are sensitive to both canopy structure and leaf characteristics, making it difficult to distinguish changes in chlorophyll content of leaves when canopy structure is variable.

Demetriades-Shah et al. (1990) suggested that second-derivative parameters calculated from the red edge region of the spectrum were largely insensitive to canopy structure and background effects, making them much more effective than SR or NDVI indices for estimation of leaf chlorosis at the canopy scale. However, the generality of those results is unclear since only one species was measured. Ongoing work in our lab confirms the utility of red edge parameters for prediction of leaf chlorophyll content from canopy reflectance but also suggests that the relationship is affected by variation in leaf thickness between species as well as changes in leaf thickness during leaf out and subsequent leaf development (Sims and Gamon 2002)

Broge & Leblanc (2000), however, found that REIP indices proved surprisingly sensitive to variations of canopy parameters, background parameters, and atmospheric parameters. **Only at high vegetation densities** did the REIP indices perform well for estimation of canopy chlorophyll concentration, where the Lagrangian interpolation method gives the most accurate estimate of REIP. It is consistently the best of the three methods for estimation of canopy chlorophyll concentration (or LAI, to be discussed later) in terms of sensitivity to canopy effects, and the best overall estimator of canopy chlorophyll at high vegetation densities.

When including LiDAR data to account for the 3D-structure of the canopies, Blackburn (2002) produced similar relationships for broadleaved canopies (i.e. exhibiting saturation effects in low and high chlorophyll concentration ranges) as in his earlier studies on leaf level; this was only modestly improved when correlating ρ_{RE} to chlorophyll concentrations per mass instead of area. Interestingly, the relationship between REIP and chlorophyll concentration (per mass) was fairly linear for coniferous stands (Blackburn 2002). It became evident that broadleaved and coniferous stands were distinctly different in terms of the relationships between their spectral reflectance and canopy characteristics, and had to be treated separately – **the typical constraint of all empirical approaches**.

Given the contradictory findings when trying to estimate canopy pigment concentration through established empirical relationships (predictive equations tend to lack robustness and portability since they strongly depend on the study area and on the experimental conditions of the reflectance acquisition) canopy reflectance models have been used as an alternative to empirical studies. Modeling investigations were originally conducted with rather simple (i.e., turbid-medium-based canopy models) (e.g. Verdebout et al. 1994). Based on a theoretical study of Jacquemoud (1993), many approaches have involved the coupling of the PROSPECT leaf optical properties model (Jacquemoud and Baret 1990) and the SAIL canopy reflectance model (Verhoef 1984), mostly applied to agricultural canopies.

A major limitation of the turbid medium models is that they do not account for some canopy architecture variables such as tree crown closure, tree density, tree heights, and shapes and dimensions of crowns, which may lead to incorrect estimation of forest reflectance. Demarez and Gastellu-Etchegorry (2000) were among the first to apply reflectance models to estimate forest canopy chlorophyll content with leaf and turbid medium canopy models coupled to a simulation of heterogeneous covers (DART) represented as realistic 3-D cell matrices. For two typical stands of the Fontainebleau Forest, characterized by very different architectures, the authors could demonstrate that this type of model necessary to retrieve realistic

chlorophyll concentrations; in comparison, turbid medium models of canopy architecture lead to less accurate estimates.

For dense and homogeneous broadleaf forest canopies ($LAI > 4$) Zarco-Tejada et al. (2001) used CASI hyperspectral imagery together with infinite reflectance and canopy reflectance models (PROSPECT & SAILH/MCRM⁸) to link leaf to canopy levels through radiative transfer simulation. Chlorophyll content was estimated by scaling-up (through spectral indices) and by numerical model inversion approaches. The study demonstrated that leaf-level relationships calculated from single leaf reflectance and transmittance data collected from the ground can be scaled-up to above-canopy level through infinite reflectance and canopy reflectance models using nominal input parameters derived for these study areas **consisting of closed canopies**. The red-edge indices and spectral and derivative indices were the best optical indices for Chl_{a+b} estimates; traditional and widely used optical indices for pigment estimation and indicators of vegetation status, such as NDVI and SR, performed poorly in the two consecutive years. These traditional indices primarily track canopy structural changes but were not able to track subtle changes due to pigment content variation. Results of SAILH and PROSPECT coupled model inversion showed comparable results to the scaling-up methodology, without the need for developing leaf-level relationships (Zarco-Tejada et al. 2001).

3.5. Leaf and Canopy Water Content

In most European countries the summer of 2003 was one of the hottest and driest on record: new temperature extremes were reached and the water deficit led to substantial losses in the agricultural production and also caused damage to forested areas. The situation was perceived as exceptional, yet it is not unlikely that the frequency and intensity of such events might increase in the future (e.g. GIEC/IPCC 2001; King 2004; Walther 2002). Earth observation systems have allowed mapping the spatial extent of areas affected in 2003, thereby providing an important perspective for land use planning under harsher climate conditions in the future (e.g. Coret 2005; Gobron 2005).

The use of spectral information to obtain information on the water status of vegetation canopies has been important in agricultural applications of remote sensing. In more recent times, under the impression of ongoing global warming tendencies, this particular information is becoming increasingly important for assessing the drought sensitivity of tree canopies as a function of species and site conditions.

⁸ Kuusk, A. (1995). A Markov chain model of canopy reflectance. *Agricultural and Forest Meteorology*, 76, 221–236.

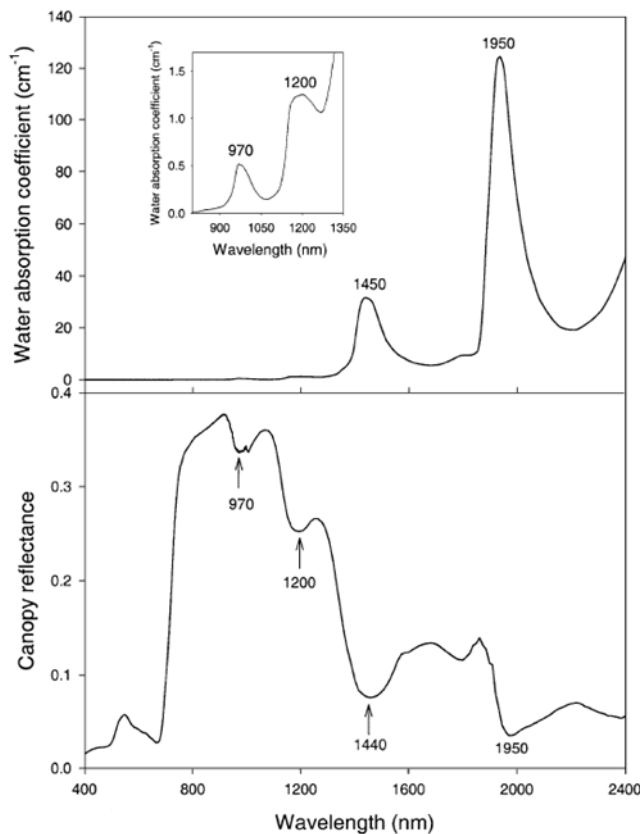


Figure 7: Water absorption coefficients and canopy reflectance (Palmer and Williams 1974; Sims and Gamon 2003).

High-resolution reflectance in the optical region has a tradition as a method for estimating plant water concentration (e.g. Carter 1991; Danson et al. 1992a; Datt 1999). Research has demonstrated strong negative correlations between reflectance in individual wavebands and leaf water content, and for single leaves, the water absorption bands in the region 1300–2500 nm showed the **highest sensitivity** to leaf water concentration (Carter 1991). However, due to quick saturation of the signal in some parts of this region, not the complete infrared range is ideal for measuring the water concentration of whole plants or canopies. Weaker absorption bands have therefore been considered more useful (figure 7), and several studies have demonstrated existing links between leaf-level reflectance in specific narrow bands in the 400–2500 nm spectral region and the amount of water in the leaf through optical indices, regression analysis and radiative transfer modeling (Aldakheel and Danson 1997; Ceccato et al. 2001; Gao 1996; Zarco-Tejada et al. 2003). In particular, the wavelengths at 1530 and 1720 nm seem to be most appropriate for assessing vegetation water (Fourty and Baret 1997), complimented by the weak liquid water absorption bands at 970 and 1200 nm (Sims and Gamon 2003).

While retrieving water content with optical methods on leaf level is quite advanced more difficulties arise when dealing with canopies. This is because the absorption features in the reflectance spectra measured by the sensor are related to the volume of leaves within a canopy as well as the water content within a leaf. The complex geometric structure of canopies implies that more advanced approaches are required than for homogeneous agricultural crops.

3.5.1. Quantifying Water Content

The degree of water stress in plants can be determined by measuring different physiological variables, such as transpiration rate or stomatal conductance, leaf water potential, or relative water content (e.g. Larcher 2002). Relative water content (RWC) is the ratio of the water volume (V) in a leaf to the maximum water volume in that leaf at full turgor (VFT), where RWC equals unity. RWC can be determined gravimetrically through

$$RWC = \frac{fw - dw}{tw + dw}$$

where fw is leaf fresh weight and dw is the leaf dry weight; tw is the weight of the water-saturated leaf at full turgor (von Willert 1995). RWC is also computed by expressing the water content as a percentage of the leaf dry weight, simply because the leaf weight at full turgor can not always be correctly determined due to the difficulty to determine the time of saturation. Since RWC is not directly tangible to optical measurements it is more efficient to relate the difference between leaf fresh and dry weight to the leaf area A:

$$EWT = \frac{fw - dw}{A}$$

EWT [g cm⁻²] stands for equivalent water thickness which defines a depth of water spread over the leaf area; in other words, EWT corresponds to a hypothetical thickness of a single layer of water averaged over the whole leaf area (Danson et al. 1992b). This concept is much closer to the physics of optical remote sensing and provides a strong conceptual foundation: departing from the Lambert-Beer absorption law, EWT can equally be expressed as

$$EWT = -\ln(1 - a)/k$$

where k is the extinction coefficient (m⁻¹) of the leaf within a spectral range that is primarily affected by liquid water absorption; a is the leaf absorptance of water and can be derived from the reflectance difference between a hydrated and a dry leaf at the same (primarily water-sensitive) wavelength. Water strongly affects the spectral reflectance of plants to some extent in the near-infrared, but much stronger in the mid-infrared region of the electromagnetic spectrum; this is the basis for the water-sensitive Leaf Water Content Index⁹ (Hunt et al. 1987)

$$LWCI = \frac{-\ln[1 - (\rho_{1.6}^D - \rho_{1.6})]}{-\ln[1 - (\rho_{1.6}^D - \rho_{1.6}^{FT})]}$$

which is based on the relation $RWC = EWT/EWT^{FT}$. The LWCI has been successfully applied to reproduce the relative water content (RWC) for leaves with negligible transmittance (fig.). Its application to morphologically different leaves might cause deviations, but it was suggested that it could be applied to plant canopies.

Another important variable related to the water content of canopies is the fuel moisture content (FMC)

$$FMC = \frac{fw - dw}{dw} 100$$

It is most commonly expressed in proportion to leaf dry weight (in percent when multiplied by 100) and may therefore have a value in excess of 1. 'Live' FMC¹⁰, i.e. the fuel moisture content of tree leaves or needles is a key variable in forest fire modeling because it is related

⁹ In both equations ρ_λ denotes the reflectance of a hydrated leaf at the given wavelength positions; superscript D refers to the reflectance of an air-dry leaf, FT to the leaf reflectance at full turgor.

¹⁰ 'dead' FMC relates to the litter on the forest floor

to the probability of ignition and to the rate of spread of a fire. When relating the dry weight of a leaf to its surface area one obtains the specific leaf weight

$$SLW = \frac{dw}{A}$$

in g cm⁻². When combining the previous equations it can be shown that FMC is related both to the amount of water in a leaf and to the amount of dry matter, i.e.

$$FMC = \frac{EWT}{SLW} 100$$

It is important to note that leaves with similar EWT may have different FMC and vice versa (Ceccato et al. 2001).

3.5.2. Spectral Indices

Tucker (1980) already suggested that the 1500-1750 nm spectral interval (the bandpass of Landsat TM Channel 5) was the best-suited band in the 700-2500 nm region for monitoring plant canopy water status from space. Some experimental studies showed that the reflectances for certain types of vegetation over the bandpass of TM Channel 5 increased as leaf water content decreased (e.g. Cibula et al. 1992). A number of broad-channel ratio and combination techniques using TM Channel 4 (0.76-0.90 µm) and TM Channel 5 were proposed for remote sensing of plant water status (Ceccato et al. 2001; Hunt and Rock 1989a; Hunt and Rock 1989b; Hunt et al. 1987; Rock 1986). Most efforts to estimate leaf water content from reflectance data have employed spectral vegetation indices that combine data in two or more wavebands. Leaf EWT has been estimated from broad waveband ratios combining NIR and SWIR wavelengths (Gao 1996; Rock 1986) or using narrow wavebands in the NIR and SWIR in simple ratios or derivatives (Ceccato et al. 2001; Danson et al. 1992a; Peñuelas et al. 1997). These indices are designed to normalize the effect on reflectance of variation in internal leaf structure, which controls internal scattering.

Laboratory measurements performed on five different leaf species (Hunt & Rock, 1989), for example, have shown a good relationship between EWT and a Moisture Stress Index

$$MSI = \rho_{16} / \rho_{182}$$

a result, which was later confirmed by a simulation study with the PROSPECT leaf reflectance model (Ceccato et al. 2001).

However, relationships often appear to be unique to individual species, and several studies using broad-channel ratio techniques failed to detect plant water status change within a biologically meaningful range. So far, no specific reference is made to high spectral resolution systems since the mentioned indices can, with some restrictions, also be applied to broadband observation systems.

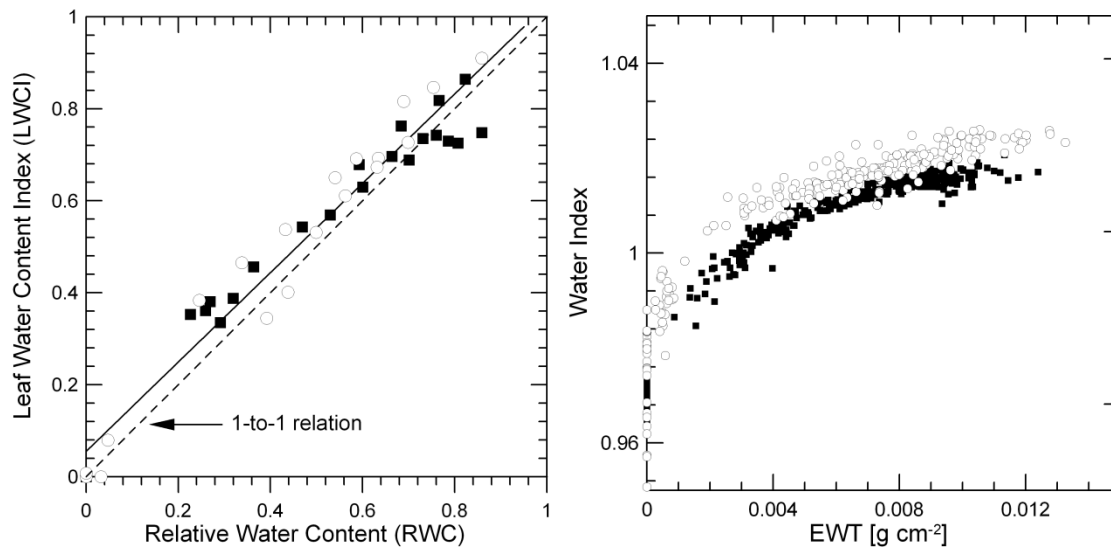


Figure 8: Experimental relationship between the relative water content and the LWCI (left), and the functional dependency of the water index (WI) of Peñuelas et al. (1997) on EWT (right), both for beech (■) and oak (○) leaves (Hill et al. submitted).

With a more specific focus on hyperspectral sensor Gao (1996) has proposed the “normalized difference water index”

$$NDWI = \frac{(\rho_{860} - \rho_{1240})}{(\rho_{860} + \rho_{1240})}$$

which is also based on classical principles for defining spectral indices: because the 1240 nm channel has similar vegetation scattering properties as the 860 nm band, and because the 1240 nm channel is sensitive to liquid water changes (figure 8), the NDWI is expected to be sensitive to vegetation liquid water changes. Peñuelas et al. (1997) have found the near-infrared region between 950 and 970 nm (where no absorption by liquid water occurs) useful for this purpose. The resulting ratio index

$$WI = \rho_{950} / \rho_{970}$$

was highly correlated with plant relative water concentration of leaves (Peñuelas et al. 1997) but in experimental studies the index was found problematic, owing primarily to a very limited value range and the resulting sensitivity to the radiometric robustness of input data; additionally, the WI appears to be sensitive to species differences (figure 8).

Classical spectroscopic techniques have been used by (Tian et al. 2001) for assessing the relative water content of wheat leaves; they obtained relationships between RWC and the depth, area and wavelength position of the 1650-1850-nm absorption feature. However, these relationships were relatively noisy, and no comparative studies on forest tree species have been identified so far.

Danson et al. (1992a) were the first to examine the usefulness of derivative spectra for assessing leaf water status. They argued that variations in leaf structure give rise to differences in leaf reflectance and may cause difficulties in relating spectral (broadband) measurements to the quantity of an absorbing medium (an effect which is of cause accounted for by selecting appropriate reference bands in spectral indices). Derivatives at eight wavelengths (corresponding to the maximum slopes on the edges of the water absorption features) were selected, and correlation analysis showed that the relationship

between EWT and the first derivative was significant at all selected wavelengths. Later the derivative approach was taken up by Pu et al. (2004) to assess the water status of infected oak leaves. They found significant relationships between RWC and derivative features from the slopes of the two strong water bands near 1400 and 1950 nm. Their practical value, however, is limited owing to the strong atmospheric effects in these waveband regions.

Ceccato et al. (2001) discuss the problems of FMC estimation from remotely sensed data and suggest that reflectance variations in the SWIR only provide information on EWT and not on FMC. However, Datt (1999) examined the relationships between EWT and FMC (referred to as gravimetric water content) and the reflectance of stacked Eucalyptus leaves and found significant correlations with EWT in the SWIR and with FMC in the NIR. In another study, Dawson et al. (1998a) trained a neural network using measured slash pine leaf stack reflectance and estimated FMC with an RMSE accuracy of 1.3% over a small FMC range from 53% to 63%; correlation between the water index (WI) and normalized difference water index (NDWI) and FMC was weaker, although no comparative RMSE estimates were given.

3.5.3. Leaf Reflectance Models

At leaf level, research using laboratory measurements and model simulations has shown that the use of reflectance measured in the optical domain can provide an estimation of leaf water content in terms of equivalent water thickness (EWT) expressed in quantity of water per unit area (g cm^{-2}) and not in terms of moisture content expressed in quantity of water per quantity of fresh or dry matter (in %). Several studies have successfully used stepwise regression and leaf reflectance model inversion to estimate leaf EWT. Leaf water dominates the spectral signature of leaves in the SWIR, and these studies have consistently observed strong correlations between leaf water content and leaf spectral response. Estimates of EWT with root-mean-square error (RMSE) accuracies of around 0.002 g cm^{-2} have been reported (Baret and Fourty 1997; Jacquemoud 2000).

When Jacquemoud et al. (1996) tested the PROSPECT leaf reflectance model on the LOPEX93 (Leaf Optical Properties Experiment) data (Hosgood et al. 1995) the concentration of water was estimated with better than 95% accuracy in fresh leaves and 54% accuracy in dry leaves. Riano et al. (2005) also accurately estimated EWT from the inversion of PROSPECT, and similar results were obtained by Hill et al. (submitted) when testing the PROSPECT model in a laboratory desiccation experiment with beech and oak leaves (figure 9). In the latter case, the numerical inversion of PROSPECT used a modified Powell's direction set method (Press et al. 1992) for simultaneously retrieving all four PROSPECT parameters (N , C_{ab} , C_w , C_m) from the reflectance spectrum, where the following search space limitations were applied: $N = 0.5\text{--}3.5$, $C_{ab} = 0\text{--}100 \text{ g cm}^{-2}$, $C_w = 0\text{--}0.05 \text{ } \mu\text{g cm}^{-2}$, $C_m = 0\text{--}0.03 \text{ g cm}^{-2}$.

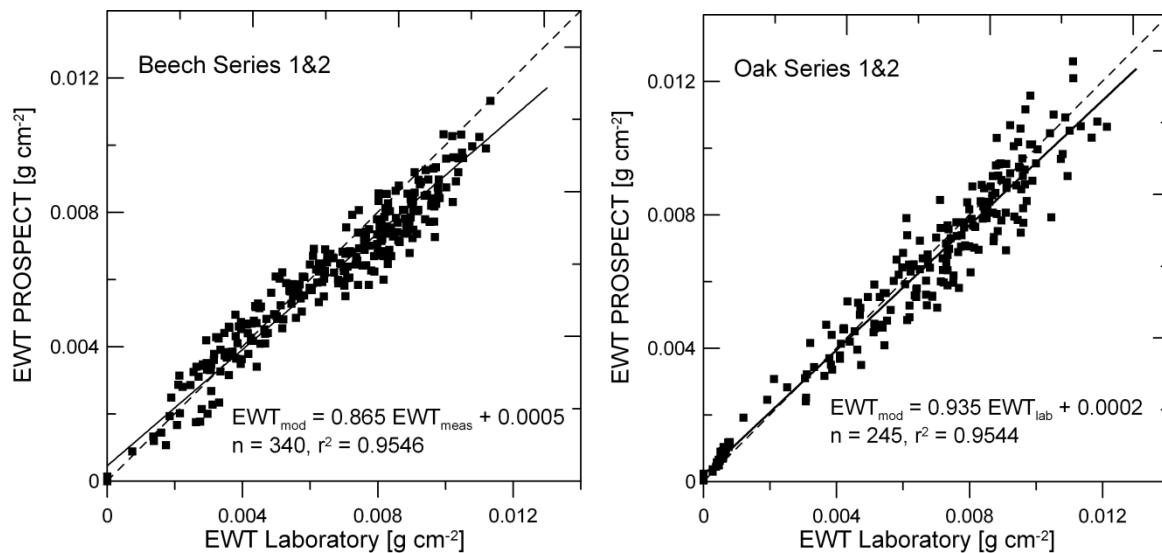


Figure 9: Retrieval of the leaf water content (EWT in g cm^{-2}) through the numerical inversion of the PROSPECT leaf reflectance model for beech and oak leaves; the dashed line represents the 1-to-1 relationship (Hill et al., submitted).

However, C_w (EWT) is not the only parameter responsible for significant reflectance variations within the SWIR range. Structural changes due to the loss of water from the cell vacuole increase the number of scattering interfaces in the palisade and spongy mesophyll and cause more intense backscattering of radiation. Therefore, a critical issue affecting the forward modelling of leaf reflectance for assessing forest canopies is the dependency of the PROSPECT leaf structure parameter N on C_w . Although an essential component for modeling the spectral response of a desiccating leaf, N cannot be directly measured. Less important for a 4-parameter-inversion (as N is one of the free parameters) variations in leaf structure have a negative impact on empirical relationships between spectral reflectance and leaf water content (Danson et al. 1992a), and Aldakheel & Danson (1997) reported an increasing mismatch between measured and modelled reflectance spectra during leaf dehydration which they attribute to changes in leaf internal structure. Jacquemoud & Baret (1990) suggested that N is related to the specific leaf area (SLA, the leaf area per unit dry weight [$\text{cm}^2 \text{mg}^{-1}$]) and proposed an empirical relationship to account for this effect. Using this relationship, however produced unrealistic results when applied to a larger variety of leaves (Ceccato et al. 2001).

Because of the absence of information about the correct relationship between N and C_w it is very difficult to take it properly into account. For this purpose, Hill et al. (submitted) conducted a dehydration experiment with beech and oak leaves and found that N varied between 1.4 and 2.5, which is in good agreement to the expected range of values for dicotyle leaves. But most importantly, the behaviour of N did not exhibit substantial species-dependant differences (figure 10). It appears thus possible to describe the co-variance between N and C_w for beech and oak leaves with a unique linear function of the type

$$N = -70.08 \text{ EWT} + 2.1156 \quad n = 585, r^2 = 0.6132$$

implying that PROSPECT can be more efficiently parameterised for simulating the leaf reflectance of pure and mixed stands of beech and oak in the forward modelling mode.

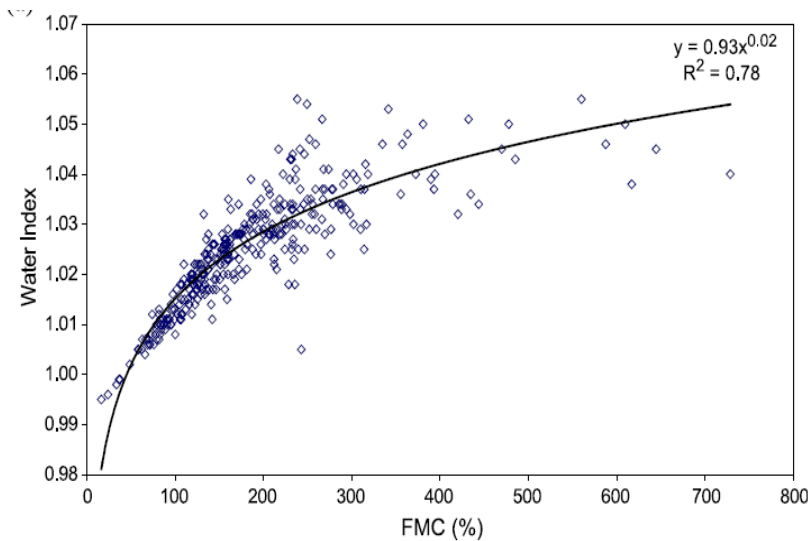


Figure 10: Relationship between the water index and fuel moisture content (FMC), PROSPECT-simulated reflectance (Danson and Bowyer 2004)

PROSPECT inversions also provided good results for dry matter (DM, r^2 of 0.85) on dry leaves, but was less successful for fresh leaves ($r^2 = 0.38$) as the higher specific absorption coefficient of water tends to mask the effect of DM on the spectral response (Riano et al. 2005). Consequently, the combination of EWT and DM retrievals did not predict FMC accurately. Danson and Bowyer (2004) also used spectral reflectance data from the Leaf Optical Properties EXperiment (LOPEX) and modelled data from the PROSPECT leaf reflectance model to examine the relationships between FMC, leaf equivalent water thickness (EWT) and a range of spectral vegetation indices designed to estimate leaf and canopy water content. Significant correlations were found between FMC and all of the selected vegetation indices for both modelled and measured data, but statistically stronger relationships were found with leaf EWT; overall, the water index (WI) was found to be most strongly correlated with FMC.

3.5.4. Scaling Up: Water Content at Canopy Level

Surprisingly few studies exist that have examined the relationships between total canopy water content and some of the leaf-related spectral reflectance indices on canopy level (e.g. Ceccato et al. 2002a; Ceccato et al. 2002b; Dawson et al. 1999; Serrano et al. 2000; Strachan et al. 2002). Indeed, when applied to canopy observations by AVIRIS, Serrano et al. (2000) found a significant correlation between the reflectance-derived WI, NDWI and the canopy RWC¹¹. However, the relationships were found to be affected not only by water content, but also by canopy structure and viewing geometry (Serrano et al. 2000), a typical effect which needs to be taken into account when open forest canopies are observed.

Sims and Gamon (2003) assumed that water content in thin plant tissues (leaves) is an efficient indicator for the varying thickness of canopies and proposed a new Canopy Structure Index

$$CSI = 2sSR - sSR^2 + sWI^2$$

with

¹¹ It should be understood that efficient and representative field sampling of RWC is a demanding task

$$sWI = \frac{(WI_{1180} - 1)}{(WI_{1180} - 1)_{\max}}$$

$$sSR = \frac{(SR_{680} - 1)}{(SR_{680} - 1)_{\max}}$$

which combines spectral indices related to structure and water content. The concept behind the CSI is that it would emphasize the Simple Ratio Vegetation Index (SR_{680})¹² when canopies were thin and would emphasize the Water Index (Peñuelas et al. 1997) at a sensitive wavelength of 1180 nm (determined experimentally) when canopies were thick (Sims and Gamon 2003). With regard to the complexity of field reference data acquisition (a precaution to be considered for all experimental approaches) the authors conclude that the CSI in fact was more sensitive to PAI¹³ than other indices, owing to its additional sensitivity to water-related absorption in plants.

In a theoretical study, Dawson et al. (1999) applied different indices and curve fitting techniques to $\log(1/\square_{\text{sim}})$ to simulated forest canopy spectra which were generated with the coupled needle reflectance model LIBERTY (Dawson et al. 1998b) and the canopy model FLIGHT (North 1996) which models conifer crowns as three-dimensional cones within a bounding box. The WI, NDWI, and chi-square curve-fitting variables were calculated for all theoretical spectra and then correlated with foliar water content, categorized by percent canopy cover and LAI. Results of the correlation coefficients indicated that the spectral indices and the chi-square curve-fitting method were robust indicators of canopy water content. However, closer examination of the relationships for the three levels of canopy cover and two LAIs indicated a reduced sensitivity and higher variability (noise) with decreasing percent canopy cover and a decreasing LAI, owing to the increasing contribution of the understory to the canopy reflectance (Dawson et al. 1999). When converting the foliar water content (fwc) used for the simulation to canopy water content¹⁴ (ct) the WI and NDWI indices exhibited strong non-linear relationships. It is obvious that these ambiguities can only be resolved when a sufficient number of corresponding spectral bands is available for separating the effects of canopy volume (LAI) and water content.

Based on earlier work Ceccato et al. (2002b) developed the global vegetation moisture index (GVMI)

$$GVMI = \frac{((\rho_{NIR} + 0.1) - (\rho_{SWIR} + 0.02))}{((\rho_{NIR} + 0.1) + (\rho_{SWIR} + 0.02))}$$

The GVMI is designed to be sensitive to water content and resistant to atmospheric effects, the NIR reflectance being rectified for atmospheric effects in a particular way by using blue reflectance (Govaerts et al. 1999; Kaufman and Tanré 1992). Retrieval of EWT_{canopy} from GVMI values is performed using a regression line derived from the model simulations:

$$GVMI = a + \frac{b}{(1 + d(EWT_{\text{canopy}}))} + c(EWT_{\text{canopy}}) - 0.13$$

(the constant 0.13 is based on available reference data; for the coefficients a, b, c and d see Ceccato et al. (2002b). The GVMI was created specifically for SPOT-VEGETATION spectral band characteristics but the theoretical approach can be used to design optimized indices for

¹² $SR_{680} = \rho_{680} / \rho_{vis}$

¹³ PAI defines the projected area of all green tissues (i.e. also non-leaf tissues) per unit ground area.

¹⁴ ct = fwc SLA LAI K_c , where SLA= specific leaf area, K_c = proportional cover)

other sensors carrying short-wave infrared, near infrared, and blue spectral bands, i.e. also for hyperspectral sensors.

Ceccato et al. (2002a) insisted that RS data provide information on vegetation moisture content expressed in terms of water quantity in the canopy per unit area (EWT_{canopy}) rather than in terms of fuel moisture content (FMC) expressed as a percentage. Other simulation studies suggested that the inversion of radiative transfer models could be used to estimate FMC, through accurate predictions of EWT and DM (Riano et al. 2005). However, the study used a much simplified turbid medium canopy reflectance model (Lillesaeter 1982), and it is to be seen whether the approach can be transferred to real canopies, where the influence of soil, understory, species mixing as well as spatial and temporal variations in leaf area index complicates the estimation.

However, most of the indices pose a problem because water stress is not only manifested in water content change but also in plant architecture change. EWT on canopy level, for example, is related to

$$EWT_{canopy} = (FM - DM) / LA,$$

where LA is the leaf area and FM and DM are the fresh and dry masses, respectively. LA, if not measured directly, can be estimated from dry plant matter as $LA = DM \cdot SLA$, where SLA is the specific leaf area (i.e. leaf area per unit of dry leaf matter). The canopy value of EWT is related exponentially to the gravimetric water content of the plant, given as a percentage of the fresh mass. EWT_{canopy} is primarily driven by changes in actual water content, which is, in turn, driven by changes in biomass. The relationship between LAI and EWT_{canopy} is inherent: EWT_{canopy} is a measure of the optical thickness of water in a stack of leaves; therefore increases in the quantity of leaves increases both the LAI and EWT_{canopy} . Therefore, radiative transfer models which incorporate the effects of viewing geometry, leaf orientation, and other descriptors of canopy complexity into reflectance might be better suited to accurately retrieve water content.

Zarco-Tejada et al. (2003) applied a combination of the PROSPECT and SAIL models, so far successfully used only for continuous agricultural canopies (Jacquemoud et al. 1996), for investigating the applicability of these radiative transfer techniques to MODIS reflectance data for vegetation water content estimation. Conceptually based on the Simple Ratio Water Index

$$SRWI = \rho_{865} / \rho_{1240}$$

they studied effects due to interactions of water content C_w , leaf dry matter C_m , leaf internal structure N and canopy LAI using the coupled models. A field sampling campaign was conducted for the analysis of FMC content, measuring fresh and dry weight from leaf samples collected in 10 study sites of chaparral vegetation between March and September. MODIS surface reflectance product MOD09A1 (500 m spatial resolution) and LAI product MOD15A2 (1 km spatial resolution) were used for C_w estimation during the period June to September 2000. Variables subject to inversion were the leaf structural parameter N , leaf dry matter C_m , and leaf equivalent water thickness C_w , with variables set to constant values in the inversion procedure ($C_{ab} = 33 \mu g \text{ cm}^{-2}$), plagiophile LADF¹⁵, and soil spectral reflectance measured in the field. Results obtained from comparing the estimated C_w by radiative transfer model inversion with the field-measured FMC content demonstrated the capability of

¹⁵ LADF: Leaf Angle Distribution Function

MODIS reflectance data to track changes of water content in vegetation ($r^2 = 0.7$ when all MODIS bands are used in the model inversion).

Again, the model combination used by Zarco-Tejada et al. (2003) is not able to account for canopy irregularities, such that also these results need to be considered with some care. With some restrictions of a limited ground data sampling Kötz et al. (2004) could demonstrate that a simple geometric leaf/canopy model (GeoSAIL) applied to hyperspectral data was successful in estimating crown forest fire fuel properties for a heterogeneous canopy like a conifer forest. The coupled radiative transfer models, PROSPECT and GeoSAIL, exploited efficiently canopy reflectance acquired by imaging spectrometry to assess quantitatively and independently the canopy structure, as well as the foliage water content of the observed forest.

3.6. Forest Canopy Structural Variables

Terrestrial vegetation controls the carbon exchange between the surface of the earth and the atmosphere. There are a plethora of local scale models that describe the cycling of carbon, water and nutrients through forest ecosystems and how these processes react to natural and anthropogenic effects. Vegetation structural variables, such as the leaf area index (LAI) are important in ecosystem models used to model the carbon cycle on different scales of operation (leaf, tree, stand, population) (Landsberg 2003). Light interception, gas exchange, photosynthesis and biomass production are all closely related to LAI (Herwitz et al. 1989 ; Nemani et al. 1993; Peterson et al. 1987), and regional variations in LAI have been found to be linearly related to site water balance (Nemani and Running 1989) and above-ground net primary production and stand volume.

Since such models often are applied over large areas on regional or national scale, the use of remote sensing data for the estimation of LAI has been the subject of many studies (e.g. Eriksson et al. 2006).

Canopy structure is generally described with only a few variables, such as the leaf area density, and the leaf inclination distribution function (LIDF). The leaf area density is defined as the total one-sided leaf area of photosynthetic tissue per unit canopy volume. The leaf area index (LAI) is then derived by integrating the leaf area density over the canopy height. Leaf area index (LAI) is a dimensionless variable and was first defined as the total one-sided area of photosynthetic tissue per unit ground surface area. For broad-leaved trees with flat leaves, this definition is applicable because both sides of a leaf have the same surface area. However, if foliage elements are not flat, but wrinkled, bent or rolled, the one-sided area is not clearly defined. The same problem exists for coniferous trees, as needles may be cylindrical or hemi-cylindrical (e.g. Jonckheere et al. 2004; Weiss et al. 2004).

The LAI is the main variable used to model many processes, such as canopy photosynthesis and evapotranspiration. It determines the size of the plant–atmosphere interface and thus plays a key role in the exchange of energy and mass between the canopy and the atmosphere. Moreover, under certain assumptions, knowledge of canopy structure variables (LAI and LIDF) allows the evaluation of the fraction of absorbed photosynthetically active

radiation (fAPAR), which is required to model the canopy's photosynthetic activity in a straightforward way. The canopy structure is also critical to the description of the canopy microclimate, which includes wind, temperature, and moisture profiles within and above the canopy that not only affect the plant itself but other living organisms, such as pathogens and insects.

For temperate forest Le Dantec et al. (2000) have compared maximum LAI, measured using the LI-COR LAI-2000 PCA, throughout 4 years and over 420 ha of a temperate forest across a range of stand structure (density, biomass, age) and site fertility (soil nutrient and water availability). LAI values ranged from 0.5 to 8 m²/m². This study has shown that maximal LAI was relatively stable between years. However, although the water stress did not affect LAI development in the current year, it reduced LAI of the following year only in stands with high LAI (above 5.5 m²/m²).

3.6.1. Leaf Area Index: Theory and Measurements

Leaf Area Index (LAI) can be estimated from field measurements using optical (Chen 1996; Welles and Norman 1991), harvest (Dûfrene and Bréda 1995 ; Fassnacht et al. 1997; Neumann et al. 1989) or allometric (Gower et al. 1999; Le Dantec et al. 2000; Rautiainen and Stenberg 2005) methods; thorough reviews have been provided by Bréda (2003) and Jonckheere et al (2004).

These indirect measurements are all based on the estimation of the contact frequency or the gap fraction (Ross 1981). Contact frequency is the probability that a beam (or a probe) penetrating inside the canopy will come into contact with a vegetative element. Conversely, gap frequency is the probability that this beam will have no contact with the vegetation elements until it reaches a reference level (generally the ground). The term "gap fraction" is often used and refers to the integrated value of the gap frequency over a given domain and thus, refers to the quantity that can be measured.

Expanding the Lambert-Beer extinction law to homogeneous plant canopies it would be possible to estimate LAI by measuring the attenuation of the incoming radiation in proportion to the optical distance, i.e. by measuring the incident (I_0) and below-canopy radiation (I); assuming a random distribution of leaves within the (homogeneous) canopy, this yields

$$I = I_0 e^{-kLAI}, \text{ i.e. } LAI = -1/k \ln(I/I_0)$$

where k is the canopy extinction coefficient and LAI the leaf area index (Bréda 2003). Using hemispherical optical measurements LAI is usually derived from inversion of gap fractions. A generalized formula (Gower et al. 1999) for relating LAI to gap fraction measurements is

$$LAI = - \frac{\ln[P_0(\theta)] \cos\theta (1 - \alpha) \gamma_s}{\Omega_E(\theta) G(\theta)}$$

where $P_0(\theta)$ is the gap fraction in the direction of the zenith angle θ ; $G(\theta)$ is the projection coefficient, or the mean projection of unit canopy element, $\Omega_E(\theta)$ is the canopy element clumping index for all levels larger than the shoot¹⁶; γ_s is the within-shoot clumping index (needle-to-shoot area ratio); α is the ratio of woody area to total element area, and $\cos \theta$ is the correction for the path length ($1/\cos \theta$) travelled by a ray of light in the direction of the

¹⁶ i.e. it describes the deviation of foliage from a random spatial distribution at scales coarser than the shoot.

zenith angle ω (Walter et al. 2003). The woody-to-total area ratio, ω , is typically calibrated by destructive sampling at each site; the needle-to-shoot area ratio, γ_s , can be estimated by analysis of shoots as described in Chen et al. (1997).

Gap fraction methods, using for example the LAI-2000 instrument or hemispherical photographs, provide the effective LAI (L_E) (Black et al. 1991), and must be corrected for both the spatial distribution of the canopy components and for the influence of the woody material. The correction from L_E to LAI can be performed using

$$LAI = \frac{(1 - \omega) L_E \gamma_s}{\Omega_E}$$

i.e.

$$L_E = LAI \frac{\Omega_E}{(1 - \omega) \gamma_s}$$

Comparing LAI derived from optical devices with the true LAI value measured with destructive sampling leads to an underestimation in the case of aggregated canopies where $\Omega_E / [(1 - \omega) \gamma_s] < 1.0$ and overestimation for regular foliage where $\Omega_E / [(1 - \omega) \gamma_s] > 1.0$ (Fassnacht et al. 1994).

In deciduous stands, the needle-to-shoot area ratio, γ_s , is set to the value of one. L_E is derived from the inversion of gap fraction measurements. Measuring gap fraction is thus equivalent to measuring transmittance at ground level, at wavelengths for which the assumption of black vegetative elements is valid (Weiss et al. 2004). This basically means that, given constant LAI, the total cumulative gap fraction increases with the tendency of clumping.

More detailed information on clumping effects in different type canopies is, for example, provided by Lacaze et al. (2002) and Lacaze and Roujean (2001) who show that conifer forest exhibit substantially higher clumping effects (ω around 0.5) than broadleaf stands (ω around 0.7-0.8). It should also be observed that in the case of indirect measurements, LAI is measured using optical instruments without considering the clumping effect. Optical instruments, such as the LAI-2000, measure canopy gap fractions from the penetration of light at various angles. These gap fraction values are then inverted to obtain LAI assuming a random spatial distribution of leaves ($\omega = 1$; see Chen et al., 1997). In this case, what is measured is in fact the effective LAI, $LAI_E = LAI \omega$ (Lacaze et al. 2002).

3.6.2. LAI Estimates through Empirical Relationships

As in other domains of extracting biophysical variables from remotely sensed data much of the work in retrieving LAI used empirical approaches to relate spectral measurements to biophysical parameters. While much work has been done with agricultural crops less has been reported on investigating the relationships between forest leaf area index and satellite or airborne imagery (Broge and Leblanc 2000; Chen and Cihlar 1996; Chen et al. 2002; Ekhlund et al. 2003; Fassnacht et al. 1997; Stenberg et al. 2004; Turner et al. 1999). Some of the most important contributions on the estimation of forest LAI from remote sensing data within the last 15 years has, for example, been compiled by Schlerf et al. (2005) and is presented in figure 11.

Most of these studies were carried out in western coniferous forests with large LAI gradients (Law et al. 2001; Running et al. 1986; White et al. 1997). In coniferous forest plantations, the ranges in LAI are usually lower and relationships between LAI and vegetation indices (VI) may be disturbed as other biophysical stand characteristics (such as stem density, canopy closure, tree height, etc.) influence the reflectance signal (Danson and Curran 1993; Treitz and Howarth 1999).

The derived empirical relationships between LAI and satellite-measured forest reflectance are useful, although the variation of atmospheric characteristics, background optical properties (i.e. understory vegetation, senescent leaves and soil), the architecture of the vegetation and angle effects (sensor and sun angles) may have significant impact on the relationships obtained.

As biomass increases and the canopy becomes more complete (i.e., LAI increases), red reflectance decreases as light is absorbed by leaf pigments (such as chlorophylls), while the NIR signal increases as more leaf layers are present to scatter the radiation upward because plant cell walls—notably the lignin component—cause scattering of NIR energy, resulting in relatively high NIR transmittance and reflectance (e.g. Gong et al. 2003). As a result of increasing shadow within intermediate canopies, there is a decrease in reflectance; this effect disappears to some extent with closing canopies.

Sensor	VI/Method	Variable	Range	N	Relation	Reference
ATM	RVI/BRA	LAI (various conifers)	1–16	18	$R^2=0.82$	(Running et al., 1986; Peterson et al., 1987)
TM	ρ_{Red}, ρ_{NIR} /BRA	LAI (aspen)	0.5–3.5	29	No relation	(Badhwar et al., 1986)
AVHRR	NDVI/BRA	LAI (various conifers)	1–13	19	$R^2=0.70-0.79$	(Spanner et al., 1990a)
TM	NDVI/BRA	LAI (various conifers)	1–16	73	$r=0.60$	(Spanner et al., 1990b)
TM	RVI/BRA	LAI (pine)	4–7	15	No relation	(Herwitz et al., 1990)
TM	NDVI/BRA	LAI (pine)	2–10	16	$R^2=0.35-0.86$, RMSE=0.74	(Curran et al., 1992)
CASI	NDVI/MLR	LAI (various conifers)	1–12	30	$R^2>0.80$, RMSE<1.0	(Gong et al., 1995)
Helicopter-borne data	REIP/BRA	LAI (spruce)	5–11	14	$r=0.91$	(Danson & Plummer, 1995)
TM	NDVI/BRA	Crown closure	0.5–3.5	22	$R^2=0.38-0.66$	Chen & Cihlar, 1996
	RVI /BRA	(various conifers)	0.05–0.85		$R^2=0.26-0.63$	
TM	RVI/MLR	LAI (various conifers)	1.0–4.5	10	$R^2=0.71$	(Fassnacht et al., 1997)
	NDVI/MLR				$R^2=0.91$	
TM	RVI, NDVI /BRA	LAI (various vegetation types)	2–15	39	$R^2=0.65-0.90$	(White et al., 1997)
TM	NDVI/BRA	LAI (various forest types)	Not specified	17	$R^2=0.15$ (all species) $R^2=0.93$ (conifers)	(Franklin et al., 1997)
TM	CRM inversion	LAI (various vegetation types)	0–7	Not specified	LAI pattern in good accordance to the land use map	(Kuusk, 1998)
TM	RSR/BRA	LAI (pine, spruce)	0.5–6.0	35	$R^2=0.55-0.70$	(Brown et al., 2000)
AVHRR	NDVI/BRA	LAI (pine, aspen, spruce)	2.0–4.0	10	$R^2=0.46$	(Boyd et al., 2000)
	VI3/BRA				$R^2=0.76$	
CASI	REIP/BRA	LAI (spruce, pine)	3–12	16	$r=0.94$	(Lucas et al., 2000)
CASI	CRM inversion	LAI (various conifers)	1.0–3.0	20	$R^2=0.51-0.86$	(Hu et al., 2000)
CASI	CRM inversion	LAI (pine)	1.0–3.0	20	$R^2=0.16-0.67$	(Fernandes et al., 2002)
TM	CRM inversion	Cover (pine)	0.1–1.0	33	$R=0.33-0.38$	(Gemmell et al., 2002)
AVHRR	RSR/BRA	LAI (various conifers)	0.5–10.5	>50	$R^2=0.62$ RMSE=1.48	(Chen et al., 2002)

Sensors: ATM—airborne thematic mapper, TM—thematic mapper, AVHRR—advanced very high resolution radiometer, CASI—compact airborne spectral imager; vegetation index (VI): RVI—ratio vegetation index, NDVI—normalised difference vegetation index, RSR—reduced simple ratio, REIP—red edge inflection point, VI3=(nIR–mIR)/(nIR+mIR); method: BRA—bivariate regression analysis, MLR—multiple linear regression, CRM—canopy reflectance model.

Figure 11: A selection of important studies on the estimation of forest biophysical variables (Schlerf et al. 2005)

As a general result, the openness of the overstory and the spatial and temporal variations of the understory vegetation in most forests pose special challenges to the retrieval of canopy leaf area index (LAI) from remotely sensed data. The results presented in Leochel et al.

(1997) show that the correlation between the canopy LAI and vegetation indices for the boreal forest stands is, in general, small with r^2 less than 0.3. Chen and Cihlar (1996) estimated the canopy LAI from the normalized difference vegetation index (NDVI) derived from TM images over the Boreal Ecosystem-Atmosphere Study (BOREAS) flux tower sites. The correlation between the retrieved LAI and the field-measured LAI was small, with r^2 of 0.5 in the late spring and 0.42 in midsummer examples of their results, suggesting that late spring images were most useful because understory had not yet fully developed yielding better correlation between overstory LAI and satellite derived indices.

While usually focused on the relationship between LAI and classical Red/NIR vegetation indices, the study of Fassnacht et al. (1997) suggested the potential of NIR/SWIR-based indices. Brown et al. (2000) demonstrated that an empirical SWIR ($\sim 1.6 \mu\text{m}$) modification to the simple ratio (SR) vegetation index, termed the reduced simple ratio (RSR), has the potential to unify deciduous and conifer species in LAI retrieval, shows increased sensitivity to LAI, and demonstrates an improved correlation with LAI in individual jack pine and black spruce canopies. Chen et al. (2002) used this index on a wide range of forest types in Canada. Supported by a substantial amount of ground data they found that the major advantages of RSR are that the difference between cover types is very much reduced so that the accuracy for LAI retrieval for mixed cover types can be improved. Additionally, the background (understory, moss cover, litter, and soil) influence is suppressed using RSR because the SWIR band is most sensitive to the amount of vegetation containing liquid water¹⁷. Their results suggest that when systematic differences among sensors are removed, it is possible to use coarse-resolution images to map the LAI distribution with acceptable errors of less than 25% (see also Fernandes et al. 2004). To achieve this accuracy, great attention should be given to sensor calibration and image processing.

The RSR approach is conceptionally in line with the work of Sims & Gamon (2003) who argued that the better transmission of short-wave radiation into vegetation canopies (in comparison to primarily absorbing wavelengths regions in the visible) makes this wavelength range more sensitive to the coupled LAI/EWT_{Canopy} interactions.

¹⁷ For agricultural crops, RSR appears to have inconsistent response to LAI changes because the SWIR channel is sensitive to the amount of liquid water in vegetation and soil, and any irrigation of the fields can modify the observed SWIR reflectance considerably. RSR is therefore not useful for agricultural fields where water management practice is unknown.

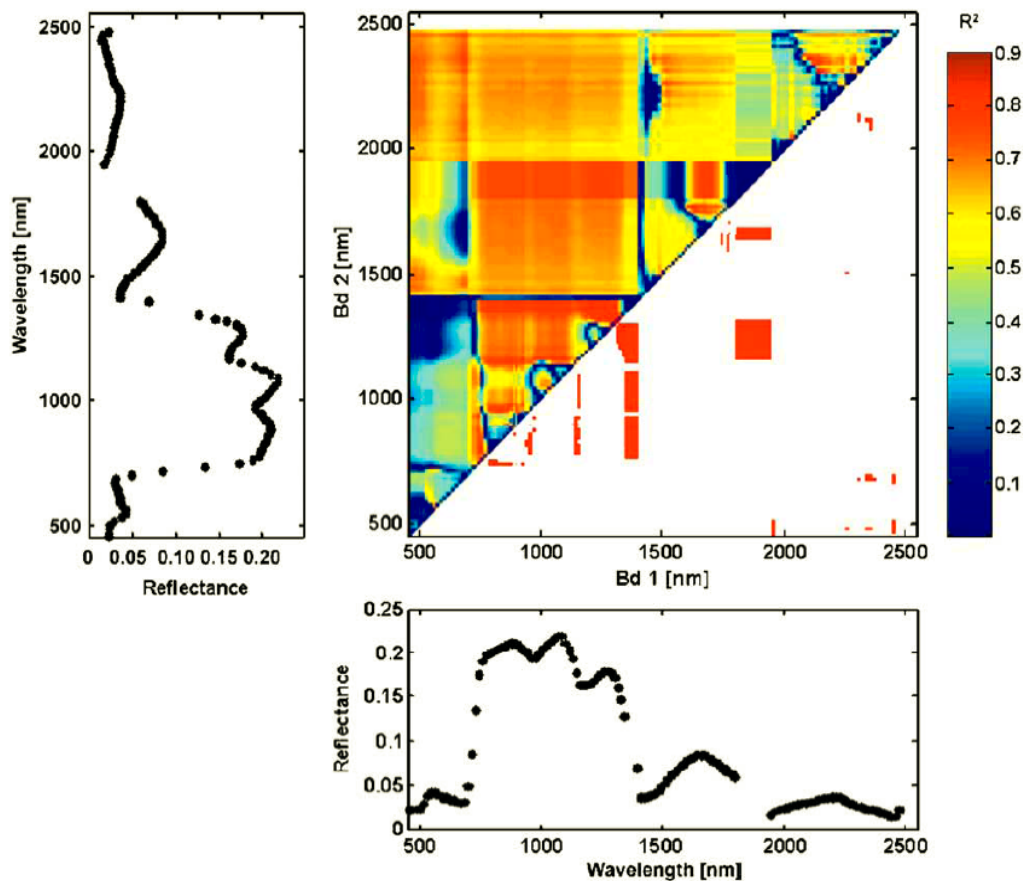


Figure 12: 2D-correlation plot showing the correlation (r^2) between LAI and values of narrow band ratio vegetation indices (RVI). The matrix is symmetrical; therefore just values above the diagonal are displayed. Below the diagonal, band combinations are marked in red where $r^2 > 0.75$. The displayed average reflectance spectrum of all measured forest plots eases the interpretation of the 2D-correlation plot. As the HyMap spectrum is not continuous, large squares of r^2 values may belong to single wavebands.

Most of the studies on forests used one or two ratio-based VI, such as the simple ratio (SR) or the normalized difference vegetation index (NDVI), computed from broadband remote sensing data (Curran et al. 1992; Herwitz et al. 1990; Peterson et al. 1987; Spanner et al. 1990a; Spanner et al. 1990b). More recently, also a systematic investigation on the performance of various broadband multispectral and **narrow band hyperspectral vegetation indices** in forests has been done.

Kooistra et al. (2008) have applied the RSR concept of Chen et al. (2002) to HyMap hyperspectral data for mapping LAI variations in softwood forest of the Netherlands. Gong et al. (2003) estimated forest LAI using vegetation indices derived from Hyperion hyperspectral data; also their results showed that that many hyperspectral bands in the SWIR region in combination with some in the NIR region have the greatest potential in forming indices for LAI estimation. The most effective band wavelengths centered near 820, 1040, 1200, 1250, 1650, 2100, and 2260 nm with bandwidths ranging from 10–300 nm. These bands are controlled by plant leaf water content, yet the absorption features by other biochemicals such as protein, nitrogen, lignin, cellulose, sugar, and starch may have indirect impacts.

Schlerf et al. (2005) systematically tested the performance of narrow-band vegetation indices for establishing relationships to LAI measurements from relatively homogenous Norway spruce stands (figure 12). Although the results were to some extent depending on stand age (structure) they found the best relationships to LAI and VOL (crown volume) when using narrow-band perpendicular vegetation index (PVI) constructed with near-infrared bands at 1088/1148 and 885/948 nm, i.e. when including water-sensitive bands in the index. A major result of their study was that the hyperspectral data set contained more information relevant to the estimation of the forest stand variables than multispectral data. Also Lee et al. (2004), who performed a comparative analysis of hyperspectral versus multispectral data for estimating LAI in four different biomes, came to the conclusion that regression models using AVIRIS channels performed better to predict LAI than those based on broadband data.

As an alternative to hyperspectral indices Hu et al. (2004) had applied the concept of linear spectral mixture analysis for the retrieval of canopy leaf area index (LAI) in three flux tower sites in the Boreal Ecosystem-Atmosphere Study (BOREAS) southern study area based on Compact Airborne Spectrographic Imager (CASI).

Linear spectral mixture analysis of multispectral and hyperspectral remote sensing data sets has been widely used in vegetation applications (e.g. Peddle et al. 1999). Hall et al. (1995), for example, employed linear spectral mixture analysis and a geometric optical model to infer the biomass density from the shadow fraction. Other biophysical parameters, such as canopy LAI, can then be derived based on their relationship with the biomass density. Using images from winter (i.e. acquired under ideally homogeneous background conditions) together with spectral endmembers of sunlit crown, sunlit snow and shadow, they found along transects that the fraction of sunlit snow was well correlated with the field-measured canopy LAI. An empirical equation was obtained to describe the relation between canopy LAI and the SMA-estimated fraction of sunlit snow (with r^2 values of 0.54, 0.71, and 0.60, respectively). CASI 2-m summer data gave less good results, likely due to the variation of the understory reflectance across the scene (Hu et al. 2004).

Whereas laboratory experiments have shown a positive relationship between the wavelength of the Red Edge Position (REP)¹⁸ and the chlorophyll content of leaf samples, canopy level experiments have met with only partial success (Curran et al. 1990). Concerning canopy structure variables (e.g. LAI) published results on the efficiency of using REP in empirical studies are to some extent diverging. Therefore, since VIs derived from the Red and NIR bands did not produce as high correlations with LAI as those with bands in the SWIR and NIR regions (Gong et al. 2003), the high correlations ($r^2=0.88$) between LAI and the red edge position (REP) which were reported by Lucas et al. (2000) are to some extent surprising but might be attributed to a highly homogeneous background situation in pine forests.

3.6.3. Background Effects

A central problem to all empirical or model-based approaches appears to be the influence of the understory in the process of estimating LAI. Rautiainen (2005), for example, compared the LAI derived from allometric estimates to that estimated by the inversion of the FRT model (Kuusk and Nilson 2000), and found that the relationship was dependent on the crown

¹⁸ i.e. red edge inflection point (REIP)

closure of the canopy; the greater the crown closure value, the stronger the correlation. A small crown closure implies that more of the understory could be seen from above, and if light is a main restricted factor for the understory vegetation cover degree, it is also an indicator of a vegetative understory (Eriksson et al. 2006). However, there are other limiting factors that could influence the cover degree of the understory vegetation, such as supply of water and nitrogen, stand age and temperature. Eklundh et al. (2001) also found that the relationship between the modeled and satellite reflectance data was considerably stronger in dense than in sparse stands, indicating an influence of the understory.

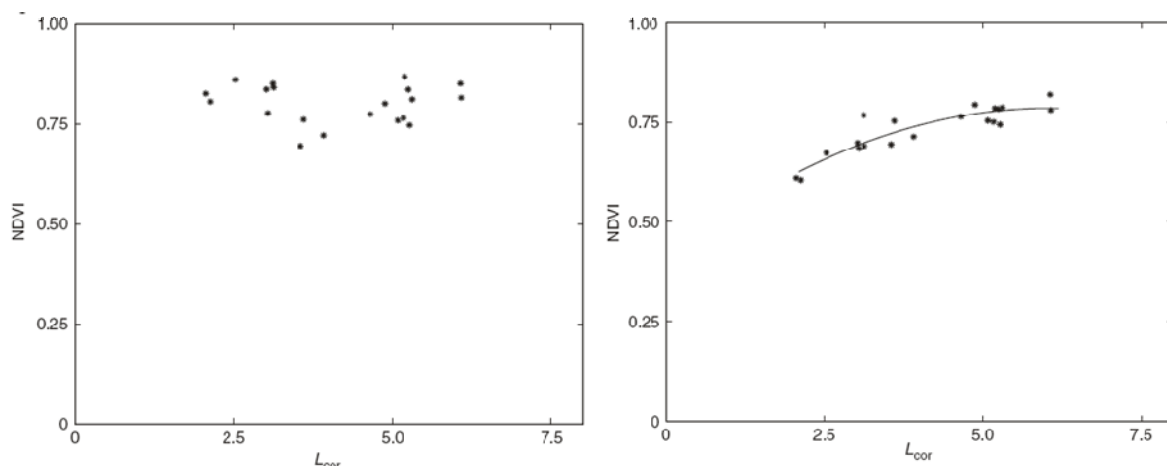


Figure 13: Comparison between LAI and NDVI (derived from modeled reflectance in the Red and NIR spectral region) without (left) and with (right) accounting for the effects of understory vegetation (Eriksson et al. 2006)

Similar as for studying leaf reflectance the use of models for generating simulated data sets with fully controlled parameter combinations has also been used in assessing structural canopy parameters. Eriksson et al. (2006), for example, have combined the PROSPECT leaf reflectance model with the FRT canopy (Kuusk 2001; Kuusk and Nilson 2000) and the 6S atmosphere model (Vermote et al. 1997) for studying the effect of understory vegetation. Knowledge concerning the understory vegetation can certainly be valuable in determining more realistic values of LAI from reflectance data; results from the simulation (figure 13) suggest that this effect can be included into model-based and empirical relationships (Eriksson et al. 2006).

Inversely, the good results reported by Hu et al. (2004) and Fernandes et al. (2002) must, to some extent, be attributed to the homogeneous background reflectance (snow cover) at the time of the CASI data acquisition.

3.6.4. Canopy Reflectance Models

Published work of Loechel et al. (1997), among others, is making it clear that simple relationships need to be replaced by canopy models for conifer boreal forests, a conclusion which also extends to broadleaf forest stands. Such model-based approaches produce interesting results such as the conclusion of Hall et al. (1996) that overstory LAI correlates best with the model-inverted shadow component of the canopy reflectance. As a result, the utility of vegetation indices for retrieving the canopy LAI for forest canopies may be very

limited, in contrast to satisfactory results obtained from the application of spectral vegetation indices to agricultural canopies (Sellers 1985, 1987).

An alternate approach to retrieval of the canopy LAI is to invert a canopy reflectance model (Goel 1988) for estimating the biophysical (and biochemical) characteristics of the canopy. The main advantage of model inversion is its general applicability to different sites and sampling conditions. A physically based approach could potentially solve many of the limitations related to empirical models if it could be shown to work accurately enough. Starting from the 1970s a number of radiative canopy reflectance models have been proposed which may be grouped according to four broad categories (Goel 1988; Roberts 2001):

Geometrical models (Li and Strahler 1985, 1992) describe the vegetation canopy using opaque geometric shapes (cones or cylinders), which cast shadows on the ground. Consequently, crown transparency is assumed to be zero. These models are mainly used to describe (sparse) forests or shrublands, where shadowing plays an important role. **Turbid medium or analytical models** (e.g. Verhoef 1984) describe the canopy as a horizontally homogenous and semi-infinite layer that contain small vegetation elements which are treated as absorbing and scattering particles of a given geometry and density. These models are better suited to describe homogenous, dense leafy canopies such as crops. However, mutual shading of tree crowns for example, cannot be taken into account. **Hybrid models** are combinations of geometrical and turbid medium models. The geometric shapes representing, for instance, tree crowns, are not considered as being opaque but are treated as a turbid medium (e.g. Huemmrich 2001). This model type is often more complex but also closer to reality. **Ray-tracing or computer simulation models** (Gastellu-Etchegorry et al. 1996; North 1996) compute the path of photons through the canopy to determine the direction of the incident rays and the direction of scattering. However, due to the complex structure and the large number of input parameters required, the latter models are difficult to invert.

Geometric-optical models, such as the Li–Strahler mutual shadow model (Li and Strahler 1992), and most hybrid geometric-optical and radiative-transfer models, such as the models developed by Li et al. (1995) and by Chen and Leblanc (1997) were developed to describe the reflectance of the properties of forest canopies. The geometric-optical models greatly simplify the calculation of the at-canopy reflectance by assuming an opaque tree crown, therefore facilitating the inversion process. Studies (Hall et al. 1995; Woodcock et al. 1997) tested the capability of the geometric-optical models in deriving the biophysical parameters of the forest canopies.

Quite sophisticated hybrid geometrical-optical and radiative-transfer models have been proposed which need a large number of physical parameters for the forest canopy (e.g. Kuusk and Nilson 2000), making inversion difficult. With the objective to avoid this complexity Huemmrich (2001) combined the SAIL model (Verhoef 1984) with the Jasinski geometric model (Jasinski and Eagleson 1989, 1990) to simulate canopy spectral reflectance and fraction of absorbed photosynthetically active radiation (fAPAR) for discontinuous canopies. This model is called the GeoSAIL model. Tree shapes are described by cylinders or cones distributed over a plane. Spectral reflectance and transmittance of trees are calculated from the SAIL model to determine the reflectance of the three components of the geometric

model: illuminated canopy, illuminated background, and shadowed background. Although the GeoSail model is relatively simple, calculations of canopy reflectance and fraction of intercepted photosynthetically active radiation (fAPAR) compared well with measurements collected in field experiments in forests in Minnesota and Oregon. The GeoSail model has been used successfully in the analysis of boreal forest landscapes (figure 14). Hall et al. (1997) used GeoSail to calculate reflectances of several different forest types over a range of canopy coverage. Kötz et al. (2004) were successful in using GeoSAIL with hyperspectral data to estimate LAI and crown forest fire fuel properties for a heterogeneous conifer canopy, and Hill et al. (2009) applied GeoSAIL for estimating LAI in Mediterranean woodlands.

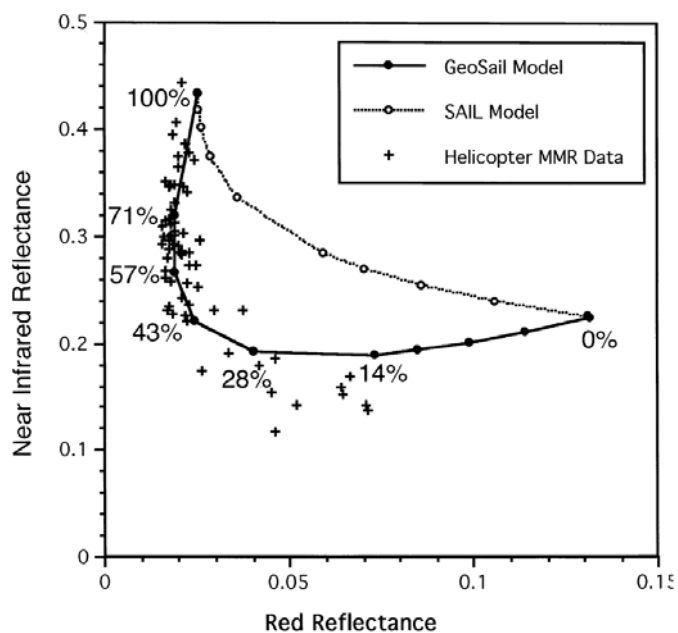


Figure14: Near-infrared and red reflectance points from helicopter measurements of aspen stands and lines for GeoSail and SAIL model results using aspen optical properties. In the GeoSail simulation, the tree shapes are cylinders. The numbers along the GeoSail line are percent canopy coverage used in the simulations for the nearest point (from Huemmrich 2001).

While GeoSAIL is limited to nadir observation geometry, Rosema et al. (1992) developed a simplified hybrid model (forest-light interaction model, FLIM). FLIM uses a geometric-optics model of photon transport between crowns and the surface and a turbid medium radiative transfer model (SAILH) for within crown photon transport, and thus accounts for both the effects of shadowing of the overstory and crown transmittance. FLIM does not explicitly include multiple scattering or mutual shadowing. However, these effects are captured to some extent in the specification of the crown reflectance. FLIM, as with many other canopy reflectance models, assumes that the field of view of the sensor contains a statistically stationary distribution of surface variables, i.e. that crowns are placed randomly and that edges between large open areas and closed canopies are not encountered.

FLIM has been applied to TM data in the Netherlands to derive LAI and canopy coverage (Rosema et al. 1992), and Gemmell and Varjo (1999) investigated the inversion of FLIM using simulated red and near-infrared reflectance data for a wide variety of stand characteristics in the boreal forest. Their results illustrate that the FLIM can be successfully inverted to retrieve the overstory crown coverage and LAI, given understory reflectance and the physical parameters of the tree crown, such as tree height and tree size.

Furthermore, FLIM inversions are limited to a field of view large enough to permit an adequate sampling of the underlying spatial distribution of surface variables; for example, a 30 m field of view is used in Hu et al. (2000). In this study, the authors produced canopy LAI and canopy closure maps for the BOREAS flux tower sites using the Compact Airborne Spectrographic Imager (CASI) winter data. With regard to the prevailing ellipticity of the tree crowns in their study site FLIM was modified to account for the effects of crown's shape on the shadows on the ground based on the approach used by Li and Strahler (1992). A strong correlation was found between the retrieved canopy LAI and the field-measured LAI along transects using this modified model with r^2 values between 0.51 and 0.86 (Hu et al., 2000).

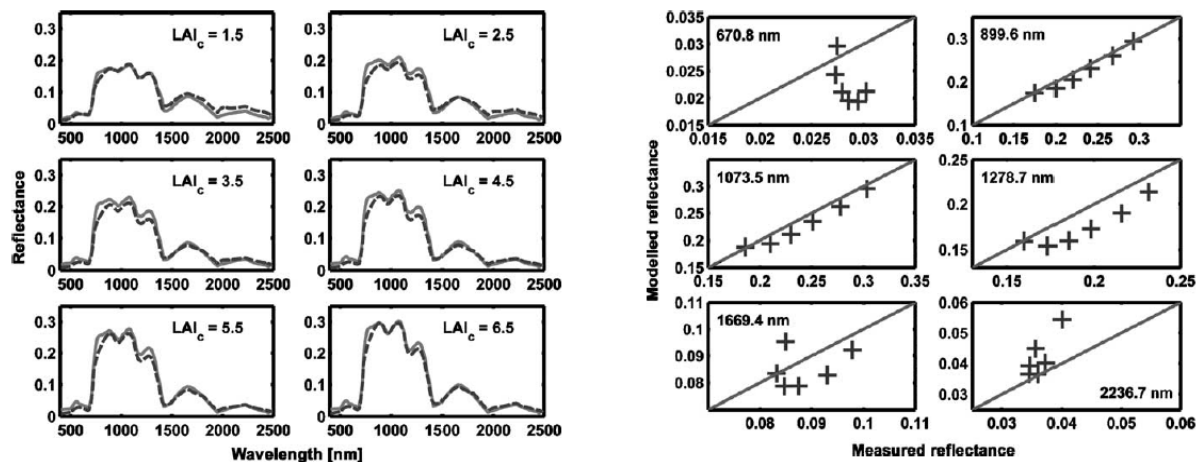


Figure 15: Measured (continuous bright line) and modelled (dashed dark line) forest canopy reflectance for certain values of canopy LAI (left) and modelled versus measured forest canopy reflectance for certain values of canopy LAI in different wavebands (right). The one-to-one line is shown for orientation (from Schlerf and Atzberger 2006).

In addition, recent enhancement of FLIM has been reported by Fernandes et al. (2002) for boreal canopies with significant clumping, such as for black spruce, through the addition of ray tracing features in a new algorithm called FLIM-CLUS. In parallel Atzberger (2000) proposed an innovative extension of the FLIM model which he named INFORM (figure 15). The INFORM concept is based on coupling FLIM with LIBERTY and SAILH, including simulated understory reflectance (Schlerf and Atzberger 2006). For broadleaf forest stands, LIBERTY can be replaced by the leaf reflectance model PROSPECT.

The main result of this study is that forest leaf area index could be estimated through inversion of the INFORM reflectance model with accuracy comparable to that of VI based approaches. These findings are supported by other studies. For instance, inversion of the hybrid-type Kuusk–Nilson model (Kuusk and Nilson 2000) performed better than NDVI when estimating forest cover from TM data, though accurate estimates on a per-stand basis were not possible (Gemmell et al. 2002). Whereas empirical approaches rely on a calibration function between a certain vegetation index and a ground measured forest variable, calibration of the reflectance model is based on synthetic data and the ground truth serves as a validation base. In opposition to empirically derived prediction functions that are generally limited to the local conditions at a certain point in time and to a specified sensor type, the calibrated reflectance model could be applied more easily to different optical remote sensing

data acquired over (managed) central European spruce forests (Schlerf and Atzberger 2006).

3.6.5. fAPAR

An important issue related to improved retrievals of LAI and, in particular, of clumping effects in the canopy, relates to estimates of the radiation budget. In the typical case of a boreal conifer forest, for example, $LAI = 3$ and $\omega = 0.5$. Assuming a random distribution and thus $G(\omega) = 0.5$, the probability of radiation penetration through the canopy at $\omega = 45^\circ$ will be 0.12 for no clumping ($\omega = 1.0$) against 0.35 for clumping ($\omega = 0.5$). In such a case, the error estimate of radiation absorption by the canopy will be above 20%. For net primary productivity (NPP), which is approximately proportional to the absorbed radiation under non-stressed conditions the error will be of the same order.

In addition to biophysical variables the physiological property of absorbed photosynthetically active radiation (APAR) can be estimated. The rate at which a green plant grows is limited by the rate at which it can assimilate CO₂ from the atmosphere for the production of carbohydrate. The energy required for this process is supplied by visible radiation, or more specifically, by quanta which are absorbed by molecules of the pigment chlorophyll which is distributed in the cells of the leaves or other green tissue (Monteith, 1981). Thus in nonwater or nontemperature limited environments the photosynthetic rate of a vegetation canopy can be limited either by the concentration of CO₂ or by the amount of APAR. In the remote sensing of vegetation, measurements of radiative flux in the visible and near-infrared portion of the electromagnetic spectrum have been used to calculate a number of vegetation indices such as the simple ratio (SR) and the normalized difference vegetation index (NDVI) (Perry and Lautenslager, 1984). NDVI has been related to the amount of green vegetation (Curran and Williamson, 1987; Curran et al., 1992) and also the amount of photosynthetically active radiation (PAR) absorbed by the green canopy (Asrar et al., 1984; Myneni et al., 1995; Riado et al., 1998). Since the growth rate of vegetation should depend on the absorbed fraction of radiation, NDVI can legitimately be used to provide an estimation of vegetation growth rate when the relation between growth and intercepted radiation is known (Monteith and Unsworth, 1990). For example, Goward et al. (1987) related integrated NDVI to net primary productivity (NPP) using energy conversion factors to convert APAR to NPP for different biome types. Additionally, algorithms using the NDVI have been used to estimate APAR for direct input into ecosystem models that predict NPP (e.g., Running et al., 1994; Field et al., 1995).

3.7. Forest Mapping, Inventory and Classification

The accurate mapping of forest community composition into distinct cover classes is essential for invoking a particular model (with a suitable set of parameters) to simulate the processes corresponding to each cover class (Hall et al. 1995; Nemani and Running 1996; Running et al. 1995). Additionally, forest structure and successional stage are key components for gap models (e.g. Shugart 1984) and for evaluating changes in an ecosystem function (Goward and Williams 1997). For example, it has been proposed that regenerating tropical forests are a major sink of atmospheric CO₂ (e.g. 2002).

Forest mapping has been achieved traditionally using spectral pattern recognition methods such as supervised classification based on the maximum likelihood decision theory (e.g. Schowengerdt 2006). Remotely sensed spectral data has been used to identify broad categories of forest cover, for example, conifer versus deciduous stands. Broad band instruments used for land cover identification include the Landsat Thematic Mapper (TM) and Multispectral Scanner (MSS), and SPOT HRV. A number of studies have used these instruments to classify forest type at a more detailed species resolution with varying degrees of success (e.g. Skidmore 1989).

Based on leaf data collected for assessing forest stand biochemistry the study of Martin et al (1998) suggested a subset of spectral bands which were statistically important in the calibration of AVIRIS spectra in determining plot-level foliar nitrogen and lignin concentration at Harvard Forest and Blackhawk Island (Martin and Aber 1997). They conclude that hyperspectral data have an increased information content and are better suited for a precise classification of forest stands than multispectral data (Köhl and Lautner 2001; Lee et al. 2004; Niemann 1995; Ustin and Xiao 2001). However, mapping tree species in the highly managed and fragmented European forest areas meets another dimension of problems. Coniferous tree plantations, for example, are characterized by very subtle differences in reflectance (figure 16), such that also hyperspectral data alone do not lead automatically to improved results (Coleman et al. 1990, Köhl and Lautner 2001).

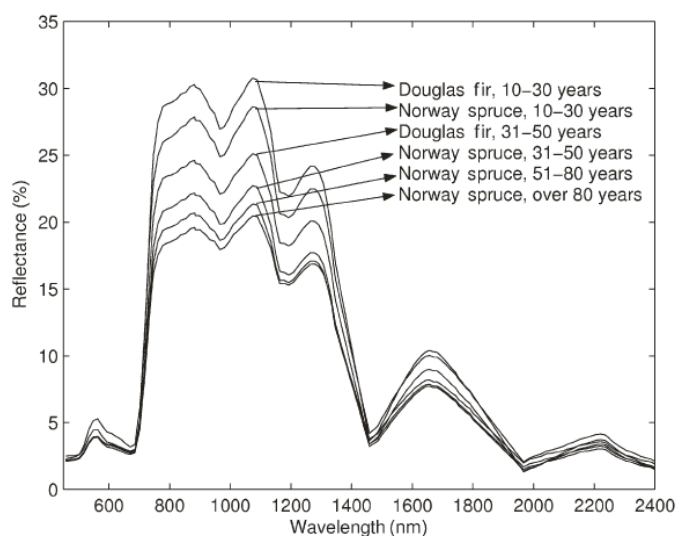


Figure 16: Mean reflectance spectra of the six classes of coniferous trees considered, from HyMap imagery (Buddenbaum et al. 2005).

An appropriate strategy to improve stand classification is to combine the spectral pattern with additional information channels. Similar to Franklin (2000), the study of Buddenbaum et al. (2005) could gain classification accuracy by including geostatistical texture parameters in the classification; pseudo-cross madograms, a newly introduced geostatistical texture measure, performed best. The classification accuracy (kappa) using hyperspectral data alone was 0.66. Application of pseudo-cross madograms increased it to 0.74 (Buddenbaum et al. 2005). Other work has successfully used digital elevation data as supplementary variable (Frank 1988).

Recent advances in classification methodologies have potential to increase the accuracy with which such forest mapping can be undertaken (e.g. Canty 2006; Martin et al. 1998). Artificial

Neural Networks and in particular new pattern recognition algorithms such as Support Vector Machines (e.g. Burges 1998; Vapnik 1995) have raised considerable attention and are certainly worthwhile to be further explored with regard to hyperspectral image classification.

However, no further much detail is discussed here because classification algorithms are dealt with in the context of a study report on general processing tasks (ToolBox) submitted by the Humboldt University Berlin.

There are not many options for using hyperspectral imagery to study biodiversity issues which cannot be investigated with traditional multi-spectral systems, in particular because spatial structure are usually preferred in comparison to high spectral resolution information. Even when taking into account the limited spatial resolution of the future EnMap system it appears feasible to take profit of the detailed spectral information content for deriving biodiversity-related information. Schmidtlein and Sassini (2004) demonstrated that continuous transitions between plant species assemblages could be modeled by extrapolating axes of an unconstrained ordination of species data. The authors also modeled the distribution of plant functional response types (Ellenberg indicator values) and the cover values of selected species. The models were made with partial least squares (PLS) regression analyses based on high-resolution hyperspectral airborne imagery.

3.8. Recommendations: Research Priorities

The need for accurate information on the status of forests and, in particular, where and how they change over time is high on the agenda (Boyd and Danson 2005). This information is required at a range of spatial and temporal scales, from local forest inventories used for economic resource management purposes and updated annually, through to global data on carbon, water and energy fluxes required for environmental management (e.g., the modeling and mitigation of climate change) over a number of decades (Cohen et al., 2001).

Although a number of studies have been presented where the use of Earth observation satellites (Landsat, SPOT) for assessing forest stand properties has been explored (e.g. Ardö 1992; Ardö et al. 1998; Brockhaus and Khorram 1992; Cohen and Spies 1992; Jensen et al. 1999; McRoberts 2008; McRoberts and Tomppo 2007; Poso et al. 1987; Tomppo et al. 2008; Wulder 1998) the review presented in this paper clearly emphasizes that optical remote sensing and hyperspectral image analysis in particular has been primarily used in the context of improving the retrieval of biophysical attributes of forest stands and ecosystems. This is and will remain important because the issue of carbon accounting under changing climate conditions will be a major issue on the political agenda within the forthcoming years. Global warming, for example, is already impacting on the existing forest management concepts, and a major research issue is to support the development of adapted management strategies by providing information on the eco-physiological sensitivity of existing tree species to changing environmental conditions (such as more frequent summery drought events, more wet and less cold winters and so forth) within a range of relevant site conditions (e.g. Lasch and Lindner 1995; Prentice et al. 1993). Since climatic effects are also triggering feedbacks on stressed tree stands, such as insect infestations and viral infections, it is important to obtain regular assessments on exhaustive spatial levels.

It is evident that remote sensing is an essential element for providing this type of information, if continuous and repeated data acquisition can be guaranteed. It is also clear that biophysical stand information derived from hyperspectral imagers needs integration with forest growth and productivity simulators (Pretzsch et al. 2007), in particular because growth cycles are extremely slow and can only be observed to a certain limit within one or two satellite generations.

However, any of the existing experimental studies are based on multispectral data, or have used only a subset of the spectral channels provided by imaging spectrometers. It is therefore recommended that the hyperspectral dimension in general needs to be further explored and exploited more intensely in forest and ecosystem applications.

A number of empirical approaches have been proposed and developed which have proved being efficient in local case studies but cannot be easily transferred to other regions and study cases. The logical consequence is to concentrate on the use of physically-based reflectance models and their inversion for retrieving the required parameters for assimilating them into forest production models. Although validation of canopy RTMs is difficult due to the complex nature of the object of interest and the difficulties to adequately sample and measure forest canopy and leaf properties, various forest canopy reflectance models have been used to estimate biophysical and biochemical variables of heterogeneous canopies with promising results (e.g. Demarez and Gastellu-Etchegorry 2000; Kötz et al. 2004; Kuusk et al. 2008; Schlerf and Atzberger 2006).

Forest reflectance models, however, involve more parameters for characterizing the highly irregular canopy structure than comparable models which are applied to agricultural crops. A major research issue is therefore to further optimize forest canopy reflectance models with regard to a manageable number of parameters (thereby reducing the risk of being trapped by ill-posed problems) which are nevertheless able to account for a wide range of deciduous and coniferous tree species.

FLIM, FLIM-CLUS and INFORM, for example, appear to offer a reasonable balance between complexity during inversion and the ability to explain spatial variations in apparent reflectance at stand (30 m) scales. Reflectance models need improvements in accounting for the effects of understory vegetation. These must be efficient, i.e. still allow for numerically stable inversion procedures. This objective is probably only achievable to an operational extent when the inversion of these models is controlled by efficient regularization strategies.

It is therefore an important research issue to establish suitable regularization schemes, for example by integrating the analysis of hyperspectral images with existing forest data bases (which in fact provide useful information on species, age, structure and volume).

This may also include testing of object-oriented versus the usual pixel-based approaches.

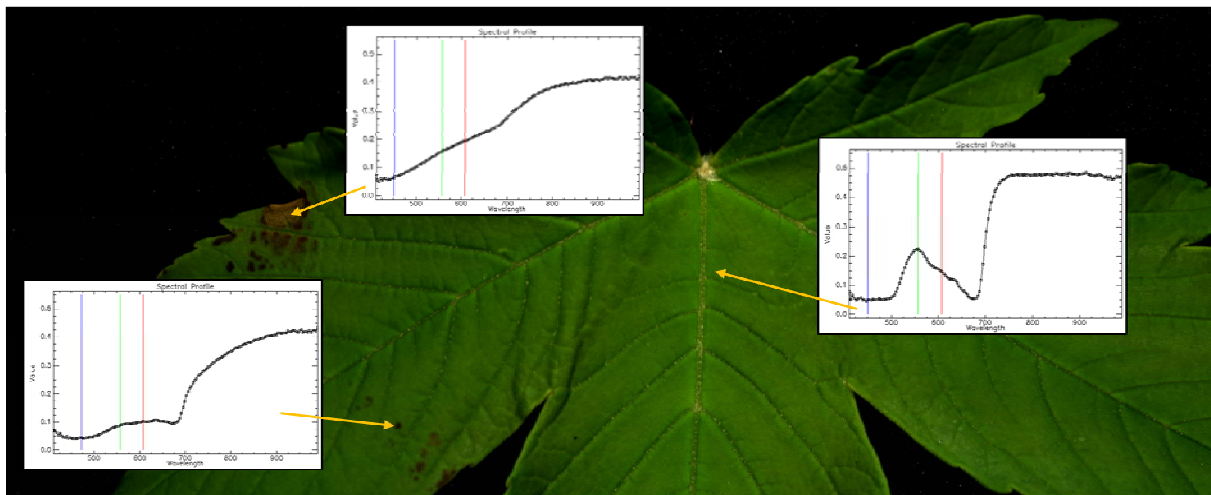


Figure 17. Hyperspectral image of an Maple leaf, showing extracted spectra from locations of undisturbed leaf development (right) as well as from two damaged areas (left). The image was acquired with a HySpex VNIR-1600 line scanner (160 spectral bands) under laboratory conditions and covers the spectral range between 400 and 1000 nm. © Remote Sensing Department, University of Trier (April 2009).

Until recent, rather little validation has been found in the literature reporting results in forest canopies from airborne or satellite-measured reflectance with ground truth. Existing validation studies need to be extended and supported by experimental hyperspectral data sets to prepare the use of operational systems when available. Particularly scaling effects between laboratory/ground and airborne/space data need to be studied more thoroughly, in particular with regard to canopy characterization and model evaluation.

Laboratory and ground measurements should be complemented with data from imaging systems which can operate on leaf and intermediate canopy level (from towers or lifters) as well as on low flying aircrafts (figure 17).

While the importance of the synergetic use of hyperspectral observations and radar data has already been emphasized (e.g. Treuhaft et al. 2003) it is also mandatory to integrate hyperspectral imaging with new types of optical sensors. Airborne laser scanners (LIDAR), for example, provide a new dimension of information on canopy structure and volume (e.g. Morsdorf et al. 2004). It will definitely be of primary importance to develop concepts for integrating canopy information from airborne LIDARs (which tend to become available on a more regular level) and microwave observations into the interpretation of hyperspectral imagers.

The integrated use of passive and active sensing might not only improve the data analysis methods but contribute to a better understanding of gaps and flaws in the existing interpretation concepts, including the improvement of geometric optics reflectance models. However, it has been emphasized in this summary paper that the acquisition of reference data on LAI, for example, is based on destructive sampling or optical measurements which are prone to considerable errors. Nowadays, high-quality ground-based laser scanners can overcome these deficits to an extent never possible before; similarly, hyperspectral imaging systems have become available for laboratory and field use (figure 17).

It is therefore a suggested research priority to support the refinement of specific data analysis components through the use of optimized data collection systems in laboratory and field experiments (preferably in existing instrumented forest monitoring sites).

Probably due to the limited availability of experimental hyperspectral data from various stages of the growing season, most of the cited work in this summary paper deals with experimental studies about biophysical parameters and ecological applications. Although these are becoming more important for optimizing forest management strategies under changing environmental conditions (see above), it is obvious that hyperspectral imaging has hardly been used for supporting operational forest management issues. While this situation is distinctly different with regard to multispectral airborne and satellite observations, it is concluded that responsible forest management institutions have been hesitating to explore the usefulness of hyperspectral imaging for regular forest inventories and surveys to a greater extent. It is therefore identified as an important research priority to explore the explanatory capacity of hyperspectral imagery for deriving management-relevant stand information (such as tree density, timber harvest volume, age/development phase and others), eventually in combination with allometric relationships and existing forest data bases.

In summary it can be stated that the combination of advanced spectral imaging technology and data analysis techniques, together with advances in remote sensing science and ecosystem modeling, have assured an important role for remote sensing in mapping, monitoring and managing forest resources. However, the true success of remote sensing will come when the results of research are transferred to organizations that have the power to use this information in deciding policy and in sustainably managing and using forest resources.

However, the regular availability of hyperspectral imagery is the major prerequisite for developing advanced application strategies.

3.9. Recommendations: Implementation (ToolBox)

Recommendations for the implementation of selected algorithms in the EnMap Toolbox are twofold and comprise simple and efficient tools as well as advanced statistical analysis and inversion methods.

Concerning the spectral indices presented and discussed in this summary no special licenses or high-level implementations are required. It will be sufficient to equip the EnMap Toolbox with an efficient mechanism for executing **spectral calculations**, using either single spectral bands or complete band arrays

These tools should be complemented by simple means required for converting and normalizing reflectance spectra (e.g. convex hull, spectral smoothing¹⁹, spectral derivatives, etc.).

¹⁹ such as the Savitsky-Golay-Filtering Algorithm

In comparison, the use of sensitive spectral bands or spectral indices for establishing empirical models by which desired target variables can be mapped (e.g. pigment concentrations, other biochemical constituents) requests the implementation of powerful statistical tools with the ability to handle large sets of collinear predictor variables and to deal with noisy patterns.

Considering the criticism expressed against multiple and stepwise regressions approaches, it is here suggested to accommodate in particular the following options:

Artificial Feed-forward Neural Networks (ANNs) as one of the standard methods in spectroscopic applications. A three-layer ANN represents an universal approximator, able to fit any continuous function, linear or non-linear, between independent and dependent variables to a pre-defined arbitrary degree of accuracy. ANNs require a learning function to adjust all the weights and biases of a given neural network. There exists a variety of different training algorithms for feed-forward ANNs, including gradient descent methods, conjugate gradient methods, the Levenberg-Marquardt algorithm (LM), to mention only a few of them.

Partial Least Squares Regression (PLSR) as an extension of the multiple linear regression and principal component regression models. PLSR projects the data into a low-dimensional space (i.e. a set of orthogonal variables, called latent variables), maximizing the covariance between the spectral matrix (X) and chemical concentration matrix (Y) by accomplishing eigendecomposition of both matrices (for detailed information. PLSR can be combined with **Genetic Algorithms** for optimizing the variable selection and thereby improving the quality of the latent variables used by PLSR.

Support Vector Machine Regression (SVM-R) as a variant that represents a different model class compared with PLSR techniques since it is based on statistical learning theory. The most valuable properties of SVMs are their ability to handle large input spaces efficiently, to deal with noisy patterns and multimodal class distributions, and their restriction on only a subset of training data in order to fit a (non-linear) function.

These advanced methods are already available through in commercial software environments (e.g. MatLab, CAMO), open-source implementations (e.g. ParLeS by R. Viscarra-Rossel, CSIRO), or routines which are published in various reference texts (e.g. Numerical Recipes²⁰). It is to be decided whether ENMap users should have direct access to these efficient algorithms inside the toolbox or via external software packages.

Concerning the **various reflectance models on leaf and canopy level** the situation is rather similar. A considerable number of sources codes (e.g. PROSPECT, SAIL, FLIM, LIBERTY, GeoSAIL, etc.) are available from the authors in direct communication with interested users. It might be useful to implement at least some core models on leaf and canopy level as integral part of the EnMap Toolbox.

²⁰ Press, W.H., Teukolsky, S.A., Vetterling, W.T., Flannery, B.P., 2007, Numerical recipes. The art of scientific computing, Cambridge University Press.

However, in case this option is pursued it must also be decided whether adequate inversion strategies are linked to the model components will be implemented as well. This, of course, renders the software implementation distinctly more complex (mainly because manifold options exist for implementing model inversions) and requires a carefully designed implementation structure.

4. Review of Algorithms with Relevance for the EnMAP Toolbox Issue – Water Remote Sensing, Short description Algorithms and Applications for the EnMAP Toolbox

B. Heim
K. Oppermann

4.1. Executive Summary

In the present document, widely accepted state-of-the-art remote sensing algorithms are presented which show the equations how to derive the chlorophyll-a concentration (5 algorithms), the Cyanobacteria abundance by its phycocyanin concentration (3 algorithms), the Suspended Particulate Matter concentration (2 algorithms), the coloured Dissolved Organic Matter concentration (2 algorithms) and the Dissolved Organic Carbon concentration (1 algorithm) from spectral reflectance data. In contrast to that, remote sensing of other optical parameters for coastal waters and inland waters still needs to be considered as experimental.

The algorithms are based on three different types of reflectance: the surface reflectance, the remote sensing reflectance and the subsurface irradiance reflectance. Equations for the transformation of the reflectances are provided.

Additionally, information on applications using hydro-optical forward- and inverse modelling is provided including the contact information of the representative European expert community. The algorithms and applications described in this document represent a selection applicable on a wide range of surface water types (inland waters, coastal waters, marine waters) and more specifically to mid-European waters.

4.2. Introduction

4.2.1. Scope

The purpose of this document is to provide a description of commonly accepted remote sensing algorithms used for surface water applications. These established algorithms have been mainly developed from hyperspectral field data sets and have then been adapted towards multi- and superspectral (e.g., SeaWiFS, MODIS, MERIS) applications. However, studies of coastal and inland waters require a high spatial resolution that is not provided by the superspectral spaceborn missions. On the other hand, the water-leaving signal is low compared to the strong signals from land surfaces, whereas the multi-spectral spaceborne missions do not provide adequate high spectro-radiometric capabilities. Therefore, the hyperspectral **EnMAP** mission will close a technical gap in water remote sensing applications.

The intended audience of the present document comprises:

- Remote Sensing Experts constructing the concept of the hyperspectral **Enmap Toolbox**
- Remote Sensing Experts applying the water application tools of the hyperspectral **Enmap Toolbox**
- Researchers from the aquatic science field for information on water remote sensing applications

4.2.2. Frequently Used Symbols and Acronyms

a_{cDOM}	absorption of coloured Dissolved Organic Matter
cDOM	coloured Dissolved Organic Matter
Chl-a	Chlorophyll-a
DOC	Dissolved Organic Carbon
EnMAP	Environmental Mapping and Analysis Program

λ	lambda
MERIS	Medium Resolution Imaging Spectrometer
MODIS	MODderate resolution Imaging Spectrometer
NIR	Near InfraRed
NN	Neuronal Network
PC	Phycocyanin
RMSE	root-mean-square-error
r^2	r-square / coefficient of determination
R_{rs}	remote sensing Reflectance
R	subsurface irradiance Reflectance
R_s	surface Reflectance
S	exponential Slope gradient
SeaWiFS	Sea-viewing Wide Field-of-view Sensor
SPM	Suspended Particulate Matter
UV	Ultra-Violet
WFD	Water Framework Directive

4.2.3. Ecological and Economical Relevance of Water Remote Sensing

There have to be extensive monitoring systems for inland and coastal waters due to their vulnerability to anthropogenic influences and global warming. Currently, eutrophication, i.e., the increase of phytoplankton biomass in aquatic systems is a major environmental problem, occurring on a global scale.

The current international classification system groups all surface water types (lakes, rivers, coastal and marine waters) under the broad **trophic categories** *oligotrophic* (low nutrients, low phytoplankton biomass), *mesotrophic* (medium nutrients, medium phytoplankton biomass), and *eutrophic* (with considerably abundant phytoplankton biomass) - with a further subdivision of the summarizing term '*eutrophic waters*': into *eutrophic*, *polytrophic* and *hypertrophic* (with rising phytoplankton abundance and the formation of harmful phytoplankton surface scum). These productive waters have a high *turbidity* due to high phytoplankton biomass. In the same way, loads of sediments make waters turbid reducing the availability of the underwater light. The monitoring of sediment loads and transport of potentially environmentally dangerous substances in coastal and fluvial systems is of major ecological and scientific relevance.

New challenges are imposed on the European national monitoring systems by the **European Union Water Framework Directive (WFD 2000)** for inland and coastal waters. **WFD** requires the member states to take actions in order to reach a good ecological status in inland and coastal waters by 2015. This involves characterization of the specific **trophic category** of aquatic systems and implementation of monitoring systems to verify the ecological status. Financial resources at the national, and local level are insufficient to assess the water quality in a timely fashion using conventional methods of regularly field and laboratory work. While remote sensing cannot replace the assessment of all relevant aquatic parameters in the field, it powerfully complements existing sampling programs and offers the base to extrapolate the sampled parameter information multi-seasonally and in space. Remote sensing technology can assist **WFD** related tasks in several ways providing spatial

and seasonal information on water quality parameters over ecologically relevant spatial and temporal scales in both coastal and inland waters.

4.2.4. Optically Detectable Water Quality Parameters

Aquatic parameters that are potentially detectable by optical remote sensing methods are:

Chlorophyll-a concentration (Chl-a),
 phytoplankton composition with focus on potentially harmful phytoplankton groups such as Cyanobacteria, floating phytoplankton mats,
 Suspended Particulate Matter (SPM) concentration,
 turbidity, Secchi depth transparency, attenuation coefficient (indicative for water clarity),
 Dissolved Organic Carbon (DOC) concentration with its water colouring fraction of coloured Dissolved Organic Matter (cDOM),
 abundance and composition of macrophytes indicative for water quality of shallow waters.

These water quality parameters are partly monitored in national and local water monitoring and management programs and are important parameters for scientific investigations. Certain aquatic water quality parameters are not optically detectable such as dissolved gases and inorganic salts.

In summary, the main functional optical parameters for water remote sensing applications are based on operational and technical aspects. The chapters 4.3.1, 4.3.2, 4.3.3, 4.3.4 focus on widely accepted methods for the remotely sensed extraction of

(4.3.1): Chl-a that is the main photosynthetic pigment abundant in all phytoplankton groups and indicative for the phytoplankton biomass.

(4.3.2): Cyanobacteria abundance that may indicate the release of aquatic toxins. Abundance can be quantified using the eutrophic-specific cyanobacterial pigment **phycocyanin (PC)** as proxy.

(4.3.3): SPM that is an important water transparency reducing component. In coastal waters, **SPM** is predominantly comprised of minerogenic particles, whereas in low-velocity inland waters, **SPM** is mainly comprised of phytoplankton.

(4.3.4): cDOM that is an important water transparency reducing component. Regionally, conversion factors transform **cDOM** into **DOC**.

4.2.5. Optical Fundamentals of Water Remote Sensing

The spectral reflectance of water is a function of its optically visible water constituents (suspended and dissolved) and the depth of the water body. Wavelengths larger than 800 nm are entirely absorbed by water so reflectance and transmission are no more significant in those longer wavelengths. As solar and sky radiation transmits into the water, the scattering by suspended particles and the absorption by suspended and dissolved water constituents (1.4) are the water colouring processes. The wavelength peak of the spectral reflectance from oligotrophic, transparent waters lies in the blue wavelength range and there is energy

reflected from the bottom up to 20 meters deep. In this case, the water-leaving reflectance may be less than 1 % of the incident radiation. The water also produces a specular reflectance directly at the water surface that may account up to 2 to 4 % reflectance. If waters are less transparent due to higher trophy or sediment loads, the spectral signal leaves the water also in the longer wavelength ranges (green to red) and there is a rise of a water-leaving reflectance even in the Near InfraRed (NIR) wavelength region. Then, the spectral information steams from a much more reduced water layer such as only from up to 1 m depth and the water-leaving reflectances may reach values of 6 %. In the case of phytoplankton blooming or high sediment loads significant water leaving signal rises in the NIR and the overall reflectance may reach near 10 to 15 %.

Natural waters are complex physical-chemical-biological media wherefore Austin (1974), Jerlov (1976) and Kirk (1983) developed hydro-optical models. The authors discriminate the optical properties that are directly measurable in the field such as the in-water hemispherical reflectance from the absorption and backscattering coefficients (Inherent Optical Properties, IOPs) that are defined to be independent of the ambient light field and are not directly measurable in the field. IOPs can be referred back up to concentrations and are measured after extraction and separation of the water constituents in the laboratory. The constituent-specific absorption (a) and backscattering (bb) coefficients are defined as coefficients per unit concentration. By adding the optical coefficients, the bio-optical frame can be adapted to specific cases such as defined by Dörffer et al. (1994), Fischer & Dörffer (1987).

Since Gordon and Brown (1973), the dimensionless **hemispherical reflectance R** is adapted to the IOPs, by

$$R = f \times \frac{bb}{a + bb}$$

Where a is the sum of the absorption coefficients, bb is the sum of the backscattering coefficients and f is an empirical factor dependent upon solar-zenith angle and volume-scattering function of the water body.

A widely used factor is defined in Morel & Prieur (1977) with $f = 0.33$. This theoretical optical framework can be used for forward and inverse modelling.

The **hemispherical reflectance, $R(z, \lambda)$** , is defined by the ratio of the upwelling irradiance, E_{up} , to the downwelling irradiance, E_{down} , both measured at the same distinct water depth, z . The required reflectance for remote sensing studies, the **subsurface irradiance reflectance, $R(0^-, \lambda)$** , cannot be measured and is calculated from the measured reflectance $R(z)$ at different depths upwards into **R** directly below the water subsurface (0^-).

For remote sensing applications, measurements of radiances and irradiances taken in water must be related to the remotely sensed above-water reflectance which is termed the **Remote Sensing Reflectance, $R_{rs}(0^+, \lambda)$** . This widely used reflectance type for water remote sensing applications is defined as the ratio of the water-leaving radiance, $L_w(0^+)$, to $E_{down}(0^+)$, directly at the water surface (0^+). To deduce **$R_{rs}(0^+)$** , $L_w(0^+)$ is calculated according to Austin (1974) using $L_{up}(0^-, \lambda)$ as:

$$L_w(0^+, \lambda) = \left(\frac{1 - r_{wa}}{n^2} \right) L_{up}(0^-, \lambda) \quad [W \cdot m^{-2} \cdot nm^{-1} \cdot sr^{-1}]$$

This formula takes into account that light is internally reflected at the water-air boundary, $(1 - r_{wa})$, where r is the Fresnel coefficient that accounts for nadir-viewing radiances for $r_{wa}0^\circ = 0.021$. In addition, the upward radiant flux is confined to a different angle, where n is the relative index of refraction of water to air, being 1.333 for fresh-water.

$$R_{rs}(0+, \lambda) = \frac{0.55L_{up}(0-, \lambda)}{E_{down}(0+, \lambda)} \quad [sr^{-1}]$$

The **Surface Reflectance**, $R_s(0+, \lambda)$, is defined as the ratio of $L_{up}(0+)$ to $L_{down}(0+)$. A part of the $L_{up}(0+)$ is always composed of directly reflected skylight, it is not possible to measure only $L_w(0+)$ by measurements above the water surface. The amount of directly *reflected skylight* varies with sun-zenith angle and water roughness, but accounts for a theoretical minimum of 2 % reflectance for a flat water surface for mid-latitude regions. Calculations according to the viewing geometries imply the Cox and Munk function (1956) depending on sky and wave conditions. Generally, in studies of turbid coastal waters and eutrophic inland waters, R_s is often directly taken, similar to land surface remote sensing applications. The positive effect of increasing water turbidity is that the intensity of the water-leaving signal becomes greater than the signal directly reflected at the water surface. Therefore, R_s has been the input parameter of a sizable number of classical water remote sensing studies on eutrophic and turbid water bodies.

Due to the low water-leaving signal, an accurate atmospheric correction is crucial for water remote sensing applications. The correction of the directly reflected skylight (skylint) from the water surface in the atmospheric correction process is needed for the retrieval of the remote sensing reflectance, R_{rs} , and the subsurface irradiance reflectance, R . The directly reflected sunlight (sunglint) from the water surface can be avoided during spectral field measurements, but has to be corrected for in airborne and spaceborne data.

4.2.6. State of Water Remote Sensing Applications

Early investigations on water clarity and suspended matter using operational satellite data were carried out, e.g. by Bukata et al. (1974), Munday & Alfoeldi (1979), or Lillesand et al. (1983) by using Landsat-Multispectral Scanner (MSS) data, but their research was radiometrically and spectrally restricted to the high water-leaving radiances from turbid and eutrophic waters. The challenge then was to extract not only relative turbidity, but to estimate the main phytoplankton pigment Chl-a from multi-spectral spaceborne data. The limited radiometric and spectral resolution of the multi-spectral sensors have not been suitable for absolute Chl-a concentrations in oligotrophic to mesotrophic waters. The average error of Chl-a derivation is high for existing multi-spectral algorithms, up to $20 \mu g l^{-1}$ Chl-a (Burgess, 2003). On the other hand, due to the limited spatial resolution ($250 m^2$ to $1 km^2$ per pixel) of the superspectral spaceborne missions (e.g. SeaWiFS, MODIS, MERIS), water quality monitoring strategies for inland waters had to be restricted to hyperspectral field spectrometry and hyperspectral airborne scanner data.

The development of water remote sensing techniques concentrates on:

Chl-a algorithms

SPM algorithms

cDOM algorithms that potentially regionally can be converted to **DOC** concentrations.

New interesting aspects are the algorithm development for the abundance of the potentially harmful phytoplankton group of **Cyanobacteria**. Also of interest are hyperspectral monitoring techniques for macrophytes and sea floor mapping (e.g. coral reefs, mussels). Algorithms of Secchi depth and attenuation coefficients exist for superspectral applications. Algorithms for phytoplankton composition, the mineralogical composition of SPM, or the geochemical composition of DOC are still in the state of research development.

Field and laboratory spectrometry and bio-geochemical investigations are essential tools to prepare useful remote sensing algorithms. Methodical standards are set in a series of NASA protocols (e.g., Fargion & Mueller (2000); Mueller & Austin (1992); Mueller & Fargion (2002)). However, methodical approaches cannot be generalized for all surface water classes of trophic state and turbidity. In non-turbid, non-eutrophic waters, the sparse scattering processes in the red-NIR are not strong enough compared to the strong water absorption and there remains no water-leaving signal. Therefore, algorithms for transparent waters are commonly restricted to the blue-green wavelength range. In contrast, red-NIR spectral analyses become possible with productive waters, because scattering on sufficiently abundant particles provide water-leaving signals at these longer wavelengths. Concentrating spectral analyses on the longer wavelengths also reduces methodological problems of above-water field spectrometry and atmospheric correction for the blue-to-green spectral wavelength range.

Commonly, successful semi-empirical algorithms are established by regression of spectral features from multi-seasonal and multi-annual field measurements. Especially, **Chl-a** algorithms are developed from comprehensive bio-optical data sets, whereas **SPM** and **cDOM /DOC** algorithms, generally, steam from limited sampling programs and data sets.

In addition to the internationally accepted semi-empirical field methodology, there exists a strong mid-European research community focusing on the development of analytical techniques to separate phytoplankton, suspended and dissolved organic matter in the water-leaving hyperspectral signal. They mainly use inverse modelling techniques involving neuronal networks NN (Dörffer & Fischer, 1994; Schiller & Dörffer, 1999; Heege & Fischer, 2004) and principal component inversion (Neumann et al., 1995; Krawczyk et al., 1996). For water studies, NN have to be trained on synthetic reflectance data sets. Real empirical NN training would be hampered by the limited availability of field data. Forward simulations offer the opportunity to provide synthetic training data with a dense and homogeneous distribution of parameters, requiring the reflectance model with specific bio-optical parameters (4.2.5). Also, forward simulations offer the opportunity for regression algorithms from synthetical data sets. The expert community for applicable NN resolutions has been contacted and is presented in chapter 4.4.

4.3. Algorithms for the Hyperspectral EnMAP Toolbox

4.3.1. Chlorophyll-a Algorithms

Phytoplankton Pigment Chlorophyll-a (Chl-a)

Phytoplankton is the autotrophic part of the plankton community. Its oxygen and primary biomass production powered by photosynthesis are of fundamental importance for the earth ecosystem. Remote sensing studies on phytoplankton predominantly seek information on the trophic category of water bodies. Phytoplankton abundance and composition is an important indicator for water quality because it relates to nutrients and light availability. The most important phytoplankton groups are diatoms (brown-greens) and dinoflagellates, Cyanophyta (blue-greens), Chrysophyta (yellow-greens), and Chlorophyta (dark-greens), all having group-specific pigment combinations. The main light absorbing pigment of all phytoplankton groups is the **chlorophyll-a (Chl-a)**. Since field and laboratory standards globally exist for **Chl-a**, and the pigment is abundant in all phytoplankton groups, the parameter **Chl-a** has been established as proxy for phytoplankton biomass.

Optical Properties

The absorption spectrum of **Chl-a** shows strong peaks at 430 nm in the blue and at 662 nm in the red wavelength range causing the greenish colour of phytoplankton-rich waters. Beyond **Chl-a**, there are accessory pigments all having different absorption bands partly overlapping each other. Chlorophyll b, c and d absorb also in the short blue and in the red wavelength range. The group of carotenoids serving as antenna pigments or antioxidants absorb in the blue-to-green wavelength range. The pigment group of phycobilins includes red pigments (e.g., phycoerythrin) and blue pigments (e.g., phycocyanin) (see under: Cyanobacterial Pigment Phycocyanin (PC)).

The spectral properties are modified by the local protein environment and by the packaging effect of the light absorbing pigments. Whereas the protein structure can slightly shift or broaden absorption features, the package effect influences absorption efficiency. Therefore, at high **Chl-a** concentrations a loss of linearity between pigment concentration and absorption efficiency occurs. Shape and magnitude of a specific absorption spectrum of one phytoplankton species may vary depending on the available wavelength range of the incident light (chromatic adaptation) and effects of stress (due to changes in nutrients, temperature, salinity). In spite of the many variables contributing, the average absorption spectra of phytoplankton communities standing for comparable temperature and nutrients regimes are remarkably constant.

Beyond absorption there are two more variables affecting the spectral reflectance: the phytoplankton scattering and the **Chl-a** fluorescence. The phytoplankton scattering varies depending on cell and colony sizes and shows lower backscattering probability with increasing cell size (Sathyendranath, 1987).

Not all light energy captured by **Chl-a** can always be used for photosynthesis. Therefore the excess of energy is either dissipated as heat or re-emitted as fluorescence. Although the total amount of **Chl-a** fluorescence is very small (only 1-2 % of the total light absorbed), the vicinity of its radiation peak at 687 nm to the **Chl-a** absorption feature in the red wavelength range may cause errors in **Chl-a** concentration calculation (Dall'Omo & Gitelson 2006).

A typical reflectance spectrum of productive waters shows minimal values in the blue wavelength range (first strong **Chl-a** absorption band) and local green and NIR reflectance maxima near 570 and 700 nm (e.g., Fig. 1, surface reflectance spectra, ZETHN and BRAMI). At around 660 to 670 nm is the local minimum (due to the second strong **Chl-a** absorption band). The reflectance peak near 700 nm rises between the red **Chl-a** absorption band and the strong absorption increase of water in the NIR. Both features (the red reflectance low and the NIR reflectance peak) shift with changing **Chl-a** concentration. Increasing **Chl-a** concentration leads to a shift of the reflectance low towards shorter wavelength ($\delta \approx 5$ nm) and of the reflectance peak towards longer wavelength ($\delta \approx 15$ nm) (Dall'Omo & Gitelson, 2006; Reigber in prep.).

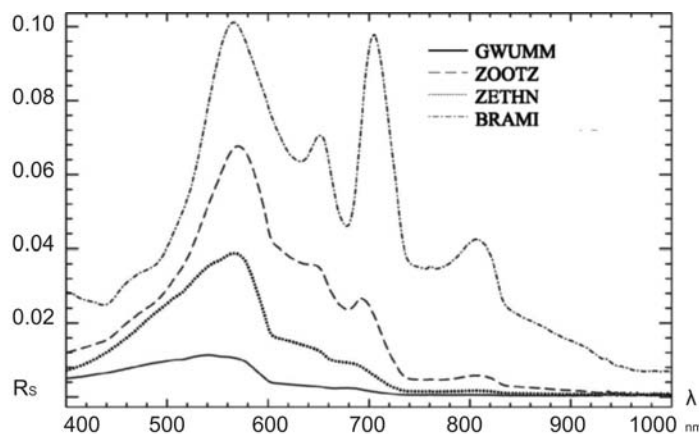


Figure 1: Surface reflectance spectra, R_s , of inland waters (Rheinsberg Lake District, Germany) representing different turbid and trophic conditions and associated in-situ Chl-a ($\mu\text{g l}^{-1}$) concentration. GWUMM, grosser Wummsee, highly transparent, oligotroph (nature reserve, densely forested); ZOOTZ, Zootzensee, mesotroph (rural, forested); ZETHN, Zethner See, turbid, mesotroph-eutroph (rural); BRAMI, Braminsee, highly turbid, polytroph (fish farming, rural) (Reigber, in prep.).

Choice of State of Art Algorithms

The recommended Chl-a algorithms are predominantly designed for applications in productive waters (Dual Band Chl-a Algorithm by Gitelson (1985); Trial Band Chl-a Algorithm by Dall'Olmo and Gitelson (2005) and Nested Band Ratio Chl-a Algorithm for MERIS by Gons et al. (2002)., case 2-eutrophic; Chl-a dependent Three Level CTL Approach by Reigber, case 2-eutrophic and case 2-coastal) where they are used for the optical monitoring of water quality. The OC4 algorithm (Ocean Colour Chl-a 4-Band Algorithm (OC4), case 1) is the operational NASA Chl-a algorithm for the oligotrophic to mesotrophic waters of the oceans and is mainly used for scientific purpose.

Dual Band Chl-a Algorithm by Gitelson (1985)

Source

The dual band ratio algorithm was introduced in 1985 by Gitelson et al. (Gitelson, A., Keydan, G., & Shishkin, V. (1985). Inland water quality assessment from satellite data in visible range of the spectrum. *Sov. Remote Sens.* 6, 28–36.) and is still one of the most

popular algorithm for estimating Chl-a concentration in case 2 waters. Here, calibration coefficients by Dall'Omo and Gitelson (Dall'Omo; G. & Gitelson, A. 2005: Effect of bio-optical parameter variability on the remote estimation of chlorophyll-a concentration in turbid productive waters: experimental results. *Applied Optics* 44, 412–422.) are used, since this most recent paper presents calibration and validation of the algorithm together with comparisons to other Chl-a algorithms.

Approach

The algorithm relates Chl-a to an absorption coefficient, which targets the absorption feature in the red at 665 nm and uses a band in the NIR at 725 nm as reference. Adjustment of this ratio by linear regression to a field data set results in a linear equation.

Formula

$$Chl - a = 70 \times a_{Chl-a} - 23$$

Where is:

$$a_{Chl-a} = \frac{R_{rs}(725)}{R_{rs}(665)}$$

Chl-a	chlorophyll-a concentration [$\mu\text{g l}^{-1}$]
a_{Chl-a}	phytoplankton absorption coefficient
$R_{rs}(665)$	remote sensing reflectance at 665 nm (respectively at 725 nm) [sr^{-1}]

Input Data

Remote sensing reflectance

Field of application

The dual band algorithm was developed for turbid productive waters (case 2-eutrophic waters). The here presented regression coefficients were derived by using a field dataset sampled in Eastern Nebraska inland waters of various settings (sand pit lakes, lakes of glacial origin, reservoirs). Data sampling was carried out in 19 field campaigns from May to October (2001 and 2002). The encountered trophic states encompass mesotrophic to eutrophic conditions (Chl-a concentrations from 5 to 200 $\mu\text{g l}^{-1}$).

Validation

Since its introduction in the eighties (Gitelson 1985), there were numerous studies applying the dual band algorithm in many different environmental conditions. However no common agreement about the right position of the chosen wavelengths could be reached. The optimal spectral bands as originally proposed by Gitelson & Kondratyev (1991) and also by Dekker (1993) are $\lambda_1=675$ nm and $\lambda_2=705$ nm. However several authors found higher correlation between Chl-a and band ratios that use a band at 675 nm in the denominator and one beyond 725 nm in the numerator (Pierson & Strömbäck 2000, Oki & Yasuoka 2002, Hoge and Wright 1987, Pulliainen et al. 2001) or that use 705 nm in the numerator and one at 665 nm in the dominator (Pierson & Strömbäck 2000, Kallio et al. 2001, Pulliainen et al. 2001, Kallio et al. 2003, Ammenberg et al. 2002). Thiemann (2000) and Thiemann &

Kaufmann (2000) established their successful Chl-a algorithm with 705 nm in the numerator and 578 nm in the denominator for northern German lowland lakes.

Parameterisation and the used data format are handled by the research community with great variability either.

Most authors preferred regression against regional datasets. Even the use of radiances instead of atmospherically corrected reflectances as done by Koponen et al. (2005) produced very good results and proves the robustness of the algorithm approach in the case of turbid, eutrophic surface waters (strong water-leaving signals).

The here presented version of the algorithm was chosen because Dall'Olmo & Gitelson (2005) based their wavelength selection on theoretical considerations about absorption properties and band positions were tested against algorithm sensitivity. In a second paper, Dall'Olmo & Gitelson (2006) investigated the algorithm for effects of parameter variability and uncertainties of reflectance measurements on Chl-a concentration estimates and finally in a third publication by Gitelson et al. (2008) comprehensive validation results are presented.

Acceptance

Accepted

Trial Band Chl-a Algorithm by Dall'Olmo and Gitelson (2005)

Source

Dall'Olmo, G., & Gitelson, A. (2005). Effect of bio-optical parameter variability on the remote estimation of chlorophyll-a concentration in turbid productive waters: experimental results. *Applied Optics* 44, 412–422.

Approach

The trial band algorithm by Dall'Olmo & Gitelson (2005) targets the Chl-a absorption maximum in the red. It sets a difference of two bands (671 nm and 710 nm) into relation to a third band (740 nm), where the band at 671 nm represents the Chl-a absorption maximum, the band at 710 nm accounts for variations in tripton and cDOM and the band at 740 nm is used as reference against total backscattering.

The slight shift of the chosen wavelength away from the absorption maximum at 675 nm is owned to interfering effects of variations of the Chl-a fluorescence quantum yield. Transformation of the resulting phytoplankton absorption coefficient to Chl-a concentrations was made by linear regression to a field data set.

The algorithm was developed by considerations about minimising interfering effects especially by Chl-a fluorescence on Chl-a concentration estimates and was directly derived from inherent optical properties.

Formula

$$Chl - a = 125 \times a_{Chl-a} + 16$$

Where is:

$$a_{\text{Chl-a}} = \left(\frac{1}{R_{rs}(671)} - \frac{1}{R_{rs}(710)} \right) \cdot R_{rs}(740)$$

Chl-a chlorophyll-a concentration [$\mu\text{g l}^{-1}$]

$a_{\text{Chl-a}}$ phytoplankton absorption coefficient

$R_{rs}(671)$ remote sensing reflectance at 671 nm (respectively at 710 and 740 nm) [sr^{-1}]

Input Data

Remote sensing reflectance

Field of application

The trial band algorithm by Dall'Olmo & Gitelson (2005) was developed for productive waters (case 2-eutrophic waters). The calibration dataset was sampled in Eastern Nebraska inland waters of various settings (sand pit lakes, lakes of glacial origin). Data sampling was carried out in 19 campaigns from May to October (2001 and 2002). The encountered trophic states encompass mesotrophic to hypertrophic conditions (Chl-a concentrations range from 5 to 200 $\mu\text{g l}^{-1}$).

Validation

When establishing the algorithm the authors provided also validation. Therefore the original field dataset was parted and 58 samples (laboratory and spectral) were used for validation.

The slope of the observed Chl-a versus the predicted Chl-a concentration was not significantly different from one, the root-mean-square-error (RMSE) was approximately 15 $\mu\text{g l}^{-1}$ and the relative RMSE was between 40 and 45%.

In a second publication about this algorithm Dall'Olmo & Gitelson (2006) modelled the influence of parameter variability and uncertainties in reflectance measurements on Chl-a concentration estimation. Adjustment of the algorithm to MODIS and MERIS band settings was done by Gitelson et al. (2008). The hereby used validation dataset (400 spectral and laboratory samples) included also samples from estuarine environment (Chesapeake Bay, USA Eastern coast).

Acceptance

New to the research community

Nested Band Ratio Chl-a Algorithm for MERIS by Gons et al. (2002)

Source

Gons, H. J. (1999). Optical teledetection of chlorophyll-a in turbid inland waters. *Environ. Sci. Technol.*, 33, 1127–1132.

Gons, H. J., Rijkeboer, M., & Ruddick, K. G. (2002) A chlorophyll retrieval algorithm for satellite imagery (Medium Resolution Imaging Spectrometer) of inland and coastal waters. *Journal of Plankton Research*, 24, 947–951.

Gons, H. J., Rijkeboer, M., & Ruddick, K. G. (2005). Effect of a waveband shift on chlorophyll retrieval from MERIS imagery of inland and coastal waters. *Journal of Plankton Research*, 27, 125–127.

Gons (1999) introduced the algorithm for shipborne optical teledetection of Chl-a. Gons et al. (2002) adapted the algorithm to MERIS band resolution assumed at this time. Gons et al. (2005) again adapted the algorithm coefficients to the finally chosen band resolution of MERIS. The formula here presented is the original one of Gons (1999).

Approach

The Chl-a red absorption peak at 672 nm is targeted in a band ratio against the NIR reflectance maximum at 704 nm. Additionally backscattering is incorporated from NIR at 762 nm. Determination of the algorithm coefficients were made by regression to laboratory Chl-a concentrations of field samples.

Formula

$$Chl - a = \frac{\frac{R(704)}{R(672)} \times [a_w(704) + b_b] - a_w(672) - b_b^p}{a^*(762)}$$

Where is:

$Chl - a$	chlorophyll-a concentration [$\mu\text{g l}^{-1}$]
$R(704)$	subsurface irradiance reflectance at 704 nm (respectively at 672 nm)
$a_w(704)$	absorption coefficient of water at 704 nm (respectively at 672 nm) $a_w(704) = 0,63 \text{ m}^{-1}$; $a_w(672) = 0,415 \text{ m}^{-1}$ (Buiteveld et al., 1994)
b_b	backscattering coefficient, assumed to be wavelength independent, derived at 776 nm
$a^*(672)$	mean specific chlorophyll-a absorption coefficient at 672 nm
p	empirical constant close to unity

Input data

Sub-surface irradiance reflectance

Field of application

The algorithm is developed for eutrophic turbid lakes and rivers and coastal waters (case 2 waters). It works best for moderate to high concentrations of Chl-a. At concentrations below $20 \mu\text{g l}^{-1}$ the algorithm underestimates Chl-a. The authors state that no region-specific calibration is necessary.

Validation

The MERIS algorithm was constructed using data collected on the IJssel Lagoon (Netherlands) in 1993–1996. Validation was performed using data on the IJssel Lagoon in 1997 and 1999, other Dutch inland waters and the Chinese Lake Tai Hu, the Scheldt Estuary (Belgium/ Netherlands) and Hudson/Raritan Estuary (New York/New Jersey), and the North Sea off the Belgian coast.

Acceptance

Accepted

Chl-a dependent Three Level CTL Approach by Reigber

Source

Reigber, S. (in prep): Erfassung limnologischer Parameter aus Gewässern des Norddeutschen Tieflandes mit hyperspektralen Fernerkundungsdaten. "Investigation of limnological parameters of inland waters in the North German Plain (Germany) using hyperspectral remote sensing data". PhD thesis, Computer Vision and Remote Sensing, Berlin University of Technology, TU Berlin.

Approach

The Chl-a dependent three level (CTL) approach was developed based on modelling and ground truth measurements. These measurements contain multi-annual and multi-seasonal (2002-2004) surface reflectance, R_s , data and the corresponding Chl-a values in the range between 1 – 290 $\mu\text{g l}^{-1}$. Spectral measurements were performed using an ASD FieldSpec. The Chl-a concentration was determined according to the German Normalization Method (DIN 38 412-L16).

By modelling and analysis of the ground truth data it could be shown that at Chl-a concentrations higher than 6 $\mu\text{g l}^{-1}$, a reflectance maximum near 700 nm appears in the surface reflectance spectrum. Furthermore, with increasing Chl-a concentration the position of the reflectance maximum near 700 nm is shifted towards longer wavelengths. This relation can be described with an exponential equation (*equation 2.5.1*). Taking into account a Chl-a range between 6 to 290 $\mu\text{g l}^{-1}$, a quantization accuracy of 7 $\mu\text{g l}^{-1}$ (RMSE) was achieved (see table below).

Considering spectral resolution limitations of hyper-spectral airborne and spaceborne sensors, the best derivation quality for Chl-a can be achieved using three different spectral features, which are optimally selected for the phytoplankton abundance. For oligotrophic to weakly mesotrophic waters with a Chl-a concentration smaller equal than 6 $\mu\text{g l}^{-1}$, the area above baseline between 650 and 685 nm ($A_{\leq 6}$) was found to be the best performing spectral feature (*equation 2.5.2*). In contrast, the area above and beneath the baseline between 665 and 757 nm ($A_{6 < \text{chl-a} < 50}$) shows the best quantization accuracy for mesotrophic to polytrophic waters with Chl-a concentrations between 6 to 50 $\mu\text{g l}^{-1}$ (*equation 2.5.3*). Finally, polytrophic and hypertrophic waters with a Chl-a concentration higher than 50 $\mu\text{g l}^{-1}$ can be analyzed based on the area above and beneath the baseline between 661 till 718 nm ($A_{\geq 50}$) (*equation 2.5.4*).

Formula

$$\text{Chl} - a_{6 < \text{chl-a} < 290} = 7.59 + 6,14e^{\frac{(\lambda - 693.9)}{4.48}} \quad 2.5.1$$

$$\text{Chl} - a_6 = 83.6 A_6 + 0.9 \quad 2.5.2$$

$$\text{Chl} - a_{6 < \text{chl-a} < 50} = -83.4 A_{6 < \text{chl-a} < 50} + 9.9 \quad 2.5.3$$

$$\text{Chl} - a_{50} = 356.71 A_{50} + 82.2 \quad 2.5.4$$

Where is:

Chl-a _{6 < chl-a < 50}	chlorophyll-a concentration with range [µg l ⁻¹]
A	Area above and below baseline
A _{≤6}	baseline for A _{≤6} 650 to 685 nm
A _{6 < chl-a < 50}	baseline for A _{6 < chl-a < 50} 665 to 757 nm
A _{≥50}	baseline for A _{≥50} 661 to 718 nm

Input

Surface reflectance

Field of application

The 3-level Chl-a algorithm is developed for three hydro-optical-trophic types of temperate lowland lakes in the Northern German lake districts: (I) oligotrophic to mesotrophic (≤6 µg l⁻¹ Chl-a), (II) meso- to polytrophic (6-50 µg l⁻¹ Chl-a), and (III) poly- to hypertrophic stage (≥50 µg l⁻¹ Chl-a).

Validation

A cross validation was performed using data (surface reflectance, Chl-a) from field campaigns in Northern German Lake districts in spring and summers 1998, 1999 (Thiemann 2000) and 2002 till 2004 (Reigber). Latter were retained for validation issues and not used during regression analysis.

Chl-a range [µg l ⁻¹]	Algorithm	R ²	RMSE [µg l ⁻¹]	Source
6 < Chl-a < 290	Position of reflectance maximum close to 700 nm	0.98	7	Reigber
6 < Chl-a < 50	Position of reflectance maximum close to 700 nm	0.98	5	Reigber
Chl-a ≥ 50	Position of reflectance maximum close to 700 nm	0.98	11	Reigber
Chl-a ≤ 6	$\int_{650nm}^{685nm} R_s(\lambda) d\lambda$	0.83	0.5	Reigber

6 < Chl-a < 50	$\int_{665nm}^{757nm} R_s(\lambda) d\lambda$	0.84	4.0	Reigber
Chl-a $\geq$ 50	$\int_{661nm}^{718nm} R_s(\lambda) d\lambda$	0.97	12.0	Reigber
1 < Chl-a < 110	705 nm / 668 nm	0.91	13.0	Thiemann (1999)
4 < Chl-a < 220	725 nm / 665nm	0.89	16.0	Dall’Olmo & Gitelson (2005)
4 < Chl-a < 220	735 nm / 673nm	0.85	18.0	Dall’Olmo & Gitelson (2005)
0.1 < Chl-a < 350	$\int_{670nm}^{750nm} R_s(\lambda) d\lambda$	0.82	20.0	Gitelson (1992)

Acceptance

New to the research community but is based on a large, multi-annual and multi-seasonal robust data set.

Ocean Colour Chl-a 4-Band Algorithm (OC4)

Source

O'Reilly, J. E., S. Maritorena, B. G. Mitchell, D. A. Siegel, K. L. Carder, S. A. Garver, M. Kahru & C. McClain (1998). Ocean color chlorophyll-algorithms for SeaWiFS. *J. Geophys. Res.*, 103(C11), 24.937–24.953.

O'Reilly, J.E., Maritorena, S., Siegel, D.A., O'Brien, M., Toole, D., Mitchell, B.G., Kahru, M., Chavez, F.P., Strutton, P., Cota, G.F., Hooker, S.B., McClain, C., Carder, K.L., Müller-Karger, F., Harding, L., Magnuson, A., Phinney, D., Moore, G.F., Aiken, J., Arrigo, K.R., Letelier, R. & Culver, M. (2000). Ocean color chlorophyll-a algorithms for SeaWiFS, OC2, and OC4: Version 4. In S.B. Hooker & E.R. Firestone (Ed.), *SeaWiFS Postlaunch Technical Report Series, Vol. 11: Seawifs Postlaunch Calibration and Validation Analyses Part 3* (pp. 9-23). NASA, Greenbelt, MD.

The OC4 is the operational NASA Chl-a algorithm designed for the Ocean Colour SeaWiFS band settings. The first version is described in O'Reilly et al. (1998) and the revised update of the 4th version in O'Reilly et al. (2000).

Approach

This approach uses the first Chl-a absorption band in the blue wavelength region. If large field data sets from oligotrophic to eutrophic waters are analysed, a sigmoidal pattern between log-transformed reflectance ratio values (blue-to-greens against maximal green wavelength range) and Chl-a concentrations becomes evident. The OC simulates this sigmoidal pattern using the SeaWiFS Bio-optical Algorithm Mini-Workshop (SeaBAM) data set (Firestone & Hooker, 1998). SeaBAM is a high quality global marine ground-truth data set

of concomitant Chl-a (fluorometric and HPLC analysis) and reflectance (in and above water) measurements from various expeditions.

Reilly et al. (1998) established from $n = 919$ SeaBAM observations the ocean colour Chl-a-2-band (OC2) and ocean colour Chl-a-4-band (OC4) algorithms. The revised updates of the 4th OC algorithm version, the OC4v4 is based on $n = 2853$ observations (O'Reilly et al., 2000)

OC4v4 performs as a 4th order polynomial with 5 coefficients and uses a switching-ratio algorithm for a wide range of chlorophyll concentrations. This maximum band ratio has the potential advantage of maintaining the highest possible satellite sensor signal to noise ratio over orders-of-magnitude range in chlorophyll concentration from about 0,01 to 60 $\mu\text{g l}^{-1}$.

Formula

$$\text{Chl} - a = 10^{(0,366 - 3,067 \text{ratioMAX} + 1,93 \text{ratioMAX}^2 + 0,649 \text{ratioMAX}^3 - 1,532 \text{ratioMAX}^4)}$$

$$\text{ratio} = \log_{10}\left(\frac{R_{rs}(443)}{R_{rs}(555)}\right), \log_{10}\left(\frac{R_{rs}(490)}{R_{rs}(555)}\right), \log_{10}\left(\frac{R_{rs}(512)}{R_{rs}(555)}\right),$$

where is:

Chl-a	chlorophyll-a concentration [$\mu\text{g l}^{-1}$]
MAX	maximal ratio
$R_{rs}(443)$	remote sensing reflectance at 443 nm (respectively at 490, 512, 555 nm) [sr^{-1}]

Input Data

Remote sensing reflectance

Field of application

The OCs are optimized for pelagic waters with oligotrophic to mesotrophic phytoplankton communities. These waters are not influenced by additional cDOM absorption or scattering processes by minerogenic SPM, and do not show reflectances in the red and NIR wavelength region.

Big lakes are similar to ocean regions in terms of underwater light climate and phytoplankton composition and therefore, the OCs also perform in oligotrophic to mesotrophic inland waters. For an OC study at the oligotrophic Lake Baikal, Siberia, Heim et al. (2005) demonstrated the performance of the OC4 within $\pm 30\%$ accuracy on multi-annual SeaWiFS data sets after a regionally adapted atmospheric correction.

Validation

The performance of OC algorithms has been evaluated in a considerable number of studies, e.g. O'Reilly et al. (2000), Gregg et al. (2004), Werdell and Bailey (2005). Generally, OC algorithms including the OC4v4 achieve accuracies within $\pm 35\%$ about the median in conditions of no atmospheric correction failure and no influences by additional cDOM absorption. The uncertainty of the Chl-a derived from satellite measurements is higher than the algorithm uncertainty since it also is affected by errors in the atmospheric correction,

sensor calibration, and other factors. Globally, the uncertainty in Chl-a OC4v4 derived from satellite measurements is $\pm 50\%$ about the median.

Acceptance

Accepted, standard NASA Chl-a algorithm

4.3.2. Cyanobacteria Algorithms

Cyanobacterial Pigment Phycocyanin (PC)

Cyanobacteria are the prokaryotic part of phytoplankton. The eucaryotic part of phytoplankton named 'algae' include all other phytoplankton groups, such as the diatoms and dinoflagellates, Chrysophyta, and Chlorophyta. Main characteristics of **Cyanobacteria** are the additional use of yellow-orange light for photosynthesis and the fixing of elementary nitrogen (Reynold & Walsby, 1975).

Cyanobacteria are of relative importance to inland water management. Under eutrophic conditions they tend to dominate phytoplankton communities and ephemeral hardly predictable algal blooms can occur. The negative effects of these mass-reproductions can be surface scum and unpleasant taste and odour in drinking water. Moreover as certain species produce cyanotoxins adverse effects to human and animal health has been reported (Backer, 2002; Pitois et al., 2000).

Optical Properties

Cyanobacteria use Chl-a as the base for photosynthesis but additionally they have a unique antenna complex containing phycobiline responsible for the extraction of energy from the yellow-orange part of light. The phycobilin pigment **phycocyanin** (PC) that is abundant in eutrophic **Cyanobacteria** species has been therefore suggested as proxy for cyan bacterial biomass (Dekker, 1993).

There are two arguments questioning this approach: First, **Cyanobacteria** adapt their internal pigment ratio to the encountered light and nutrient conditions (Tandeau de Marsac & Houmard, 1988; Lemasson et al., 1973). This process is known as complementary chromatic adaptation. Second, light absorption does not necessarily behave linear to pigment concentration. It also depends on packaging of pigments. Both effects result in highly variable specific absorption coefficients at inter- and intra-species level (Kirk, 1994; Morel, 2001; Simis et al., 2005).

Recent field studies at Dutch and Spanish lakes by Ruiz-Verdu et al. (2008) principally confirmed these findings. PC / Chl-a ratios rarely exceeded 2.5 in the Netherlands, while ratios above 4 were regularly observed in Spain. However, ratios compared only for Dutch or Spanish lakes proved fairly stable supporting the use of **PC** for the estimation of cyan bacterial biomass on a regional scale.

The diagnostic absorption feature for **Cyanobacteria** caused by **PC** is easily identified as an enhanced trough (*Fig.2*) in reflectance spectra between 600 and 650 nm (Dekker et al., 1991; Gons et al., 1992; Jupp et al., 1994; Kutser et al., 2006). Its centre was measured on extracted pigments (in vitro) in the laboratory at around 615 nm (Bryant, 1981). However in field studies (in vivo) the absorption centre has been observed between 620 and 625 nm

(Schalles & Yacobi, 2000; Dekker 1993; Simis et al., 2005). As **Cyanobacteria** always contain Chl-a as main pigment group, a cyan bacterial specific absorption spectrum will always show features of both pigments **PC** and Chl-a.

Chl-a, b and c all have secondary absorption features in the same spectral region making the use of the phycocyanin absorption feature for direct estimation of **PC** concentration more difficult. Chlorophyll b, present in green algae, has a broad maximum around 650 nm and a secondary around 600 nm, the diatom Chlorophylls c1 and c2 have secondary absorption maxima around 590 nm and 640 nm (Ficek et al., 2004; Jeffrey et al., 1997; Sathyendranath et al., 1987). Chl-a, present in all phytoplankton as the main photosynthetic pigment, has an absorption shoulder centred around 623 nm (Bidigare et al., 1990; Ficek et al., 2004; Sathyendranath et al., 1987).

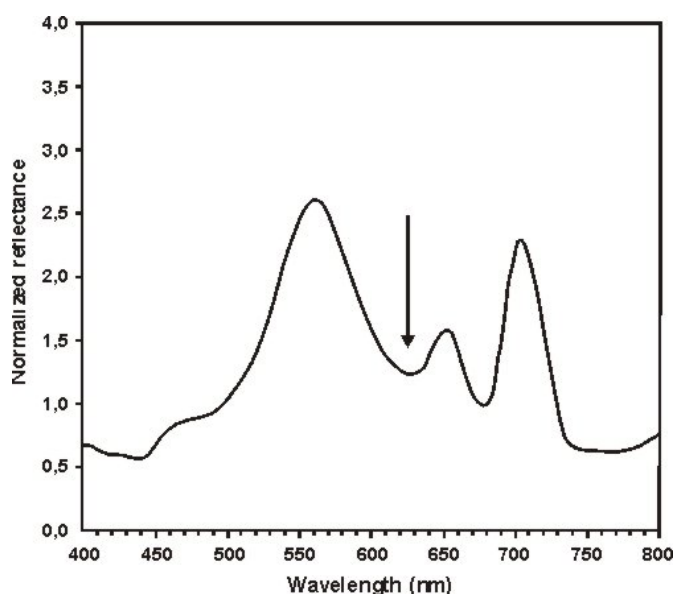


Figure 2: Reflectance spectrum normalized at 675 nm, measured in Spanish water bodies where a single species of Cyanobacteria (*Limnithrix* sp.) accounted for more than 95% of phytoplankton biomass (Ruiz-Verdu, 2008). Arrow indicates the phycocyanin absorption feature.

Choice of State of Art Algorithms

There exists a sizable number of qualitative Cyanobacteria algorithms using the relative abundance. In fact, the parameter PC is not routinely measured in the field, and laboratory routines for phycocyanin derivation from water samples are considerable elaborated. Therefore, only few Cyanobacteria algorithms calculate the Phycocyanin concentration. We present a choice of these quantitative Cyanobacteria algorithms. All Cyanobacteria algorithms are designed for water quality applications in productive waters.

Band Ratio PC Algorithm by Schalles & Yacobi (2000)

Source

Schalles, J. F. & Yacobi, Y. Z. (2000). Remote detection and seasonal patterns of phycocyanin, carotenoid and chlorophyll pigments in eutrophic waters. *Archiv fur Hydrobiologie Special Issues Advances in Limnology*, 55, 153–168.

Approach

The reflectance band ratio algorithm is based on an empirical relationship between the ratio of reflectances at $\lambda_1=650$ and $\lambda_2=625$ nm and PC concentration, obtained from a four-year study in Carter Lake, a hypereutrophic floodplain lake in Nebraska, USA. The algorithm uses reflectance at 650 nm as reference, and then targets the PC absorption at 625 nm.

Formula

$$PC = \left(\frac{R_{rs}(650)}{R_{rs}(625)} - 0,97 \right) \times 1096,5$$

where is:

PC Phycocyanin [$\mu\text{g l}^{-1}$]

$R_{rs}(650)$ remote sensing reflectance at 650 nm (respectively 625 nm) [sr^{-1}]

Input data

Remote sensing reflectance

Field of application

The reflectance band ratio algorithm was developed for turbid, shallow, eutrophic temperate lakes, in central USA. It works best for Cyanobacteria dominated phytoplankton communities with phycocyanin values between 50 and 200 $\mu\text{g l}^{-1}$. Highest errors were observed for values below 50 $\mu\text{g l}^{-1}$. When phycocyanin concentration was higher than 200 $\mu\text{g l}^{-1}$ systematic underestimation and for moderate concentrations slight overestimations occurred. Errors principally increase when other taxonomic groups than Cyanobacteria are present. The most negative effect of pigments with overlapping absorption features has been accounted for Chl-*a*. In comparison to the baseline algorithm by Dekker (1993) (2.2.3) and the nested band ratio algorithm by Simis et al. (2005) (2.2.4), errors produced with the single reflectance ratio algorithm were generally larger, while it was least sensitive to instrumental errors affecting the absolute value of reflectance (Ruiz-Verdu et al. 2008).

Validation

The reflectance band ratio algorithm has been applied to hyperspectral CHRIS-PROBA data (Ruiz-Verdu et al., 2005). It also has been applied to large set of spectroradiometric samples in combination with pigment analysis (480 samples) of lakes in the Netherlands and Spain (Ruiz-Verdu et al., 2008)

Acceptance

Accepted

Baseline PC Algorithm by Dekker (1993)**Source**

Dekker, A. G. (1993). Detection of optical water quality parameters for eutrophic waters by high resolution remote sensing. PhD Thesis. Amsterdam: Vrije Universiteit.

Approach

The baseline approach uses two wavelengths (600 and 648 nm) to draw a reference baseline, and relates phycocyanin concentration to the distance from the midpoint of the

baseline to the reflectance at 624 nm. The algorithm coefficients are based on averaged specific absorption coefficients from 10 shallow eutrophic lakes in The Netherlands.

Formula

$$PC = -24,6 + 13686 \times \{0,5 \times [R(600) + R(648)] - R(624)\}$$

where is

PC Phycocyanin [$\mu\text{g l}^{-1}$]

R(600) sub-surface irradiance reflectance at 600 nm (respectively at 648 and 624 nm)

Input data

Sub-surface irradiance reflectance

Field of application

The baseline algorithm was developed for turbid, shallow, eutrophic temperate lakes, in The Netherlands. An evaluation of this algorithm by Ruiz-Verdù et al. (2008) at lakes in Spain and the Netherlands could demonstrate best predictions in a range of phycocyanin concentrations corresponding to eutrophic conditions between 50 and 200 $\mu\text{g l}^{-1}$. The algorithm produced moderate constant relative errors of underestimation in this interval. Higher errors were found for waters with either low or very high phycocyanin concentrations. When Cyanobacteria formed the dominant phytoplankton group the accuracy of the algorithms was clearly higher, while the presence of other taxonomic groups led to increased errors. High Chl-a concentrations had the most negative effect and lead to overestimation of phycocyanin. Errors in the Spanish samples suggest that regional parameterization of the algorithm could improve its performance. In comparison to the band ratio PC algorithm by Schalles & Yacobi (2000) (2.2.2) and the nested band ratio algorithm by Simis et al. (2005) (2.2.4) the baseline algorithm was most prone to differences in reflectance caused by the measurement protocols.

Validation

The baseline algorithm has been applied to hyperspectral Hyperion data (Kutser et al., 2006) and to large set of spectroradiometric samples in combination with pigment analysis (480 samples) of lakes in the Netherlands and Spain (Ruiz-Verdu et al., 2008)

Acceptance

Accepted

Nested Band Ratio PC Algorithm by Simis et al. (2005)

Source

Simis, S.G.H., Peters, S.W.M., & Gons, H.J. (2005). Remote sensing of the cyan bacterial pigment phycocyanin in turbid inland water. *Limnol. Oceanogr.*, 50, 237–245.

Approach

The nested band ratio algorithm was developed for MERIS and relates phycocyanin to the absorption coefficient at the band centred at 620 nm, which is retrieved from the ratio of the 620 nm band and a NIR band, centred at 709 nm, as reference. A second, nested ratio (709/665 nm bands) is used to infer a correction for absorption by chlorophyll-a in the 620 nm band.

A fourth band (centred at 779 nm) is used to calculate the backscattering coefficient that is introduced in the two ratios, to retrieve the absorption coefficients through inversion of a reflectance model according to Gordon et al. (1975) and as described in detail in Gons et al. (2005).

Formula

$$PC = 170 \times \left\{ \left[\frac{R_{rs}(709) \times (0,727 + b_b)}{R_{rs}(620)} - b_b - 0,281 \right] - [0,24 * a_{ph}(665)] \right\}$$

where is

$$a_{ph}(665) = 147 \times \left[\frac{R_{rs}(709) \times (0,727 + b_b)}{R_{rs}(665)} - b_b - 0,401 \right]$$

$$b_b(779) = 1,61 \times \frac{R_{rs}(779)}{0,082 - 0,6 * R_{rs}(779)}$$

where is

PC	Phycocyanin [$\mu\text{g l}^{-1}$]
$R_{rs}(620)$	remote sensing reflectance at 620 nm (respectively at 665 nm, 709 nm and 779 nm) [sr^{-1}]
b_b	backscattering coefficient derived from $R_{RS}(779)$
a_{ph}	Chlorophyll-a absorption coefficient derived at 665 nm

Input data

Remote sensing reflectance

Field of application

The nested band ratio algorithm was developed for turbid, shallow, eutrophic temperate lakes, in the Netherlands. An evaluation of this algorithm by Ruiz-Verdú et al. (2008) at lakes in Spain and The Netherlands could demonstrate best predictions in a range of phycocyanin concentrations corresponding to eutrophic conditions between 50 and 200 $\mu\text{g l}^{-1}$. Higher errors were found for waters with either low or very high phycocyanin. At concentrations lower than 50 $\mu\text{g l}^{-1}$ the algorithm showed a tendency to overestimate and at very high concentrations to underestimate phycocyanin. In comparison with the band ratio PC algorithm and the baseline PC algorithm, the nested semi-empirical band ratio algorithm shows the best predictions of all three algorithms especially at very high phycocyanin concentrations.

However it fails when surface scum is present. When Cyanobacteria formed the dominant phytoplankton group the accuracy of the algorithms was clearly higher, while the presence of other taxonomic groups led to increased errors. Overestimation of phycocyanin mainly occurred in the presence of chlorophylls b and c, and phaeophytin (Simis et al., 2007)

Validation

The nested band ratio algorithm has been applied to MERIS imagery of inland waters (Simis et al., 2005) and to a large set of spectroradiometric samples in combination with pigment analysis (480 samples) at lakes in the Netherlands and Spain (Ruiz-Verdu et al., 2008). Simis et al. (2007) evaluated the influence of various phytoplankton pigments on the performance of this algorithm.

Acceptance

Accepted

4.3.3. Suspended Particulate Matter Algorithms

Suspended Particulate Matter (SPM)

The term **Suspended Particulate Matter (SPM)** comprises the whole of particles in the water column. **SPM** influences the light conditions of under-water ecosystems and is therefore a fundamental water quality parameter. **SPM** is also often the carrier of heavy metals and micro-pollutants such as Polychlorinated Biphenyls (PCBs) that is a class of highly toxic cancer-causing organic compounds. In river mouths and tidal areas, water remote sensing for **SPM** can be used for dynamic analyses of sediment deposition and relocation.

Total Suspended Matter, (TSM), and **seston** are synonymously to **SPM**. **SPM** without phytoplankton is the group of non algal particles (NAP), synonymously to tripton or detritus. NAP can further be subdivided in organic and inorganic particles. Organic particles are algal fungi and spores, bacterioplankton, zooplankton and dead organic matter. Commonly, phytoplankton and organic NAP dominate the **SPM** in low energy water bodies such as lakes. Whereas, abundance and transport of the minerogenic **SPM** fraction is bound to the higher-energetic rivers and coastal regions. The composition of inorganic particles (silica-oxides, aluminosilicates, iron-, and manganese-oxides and -hydroxides, clays, and calcite/dolomite) is dependent upon the lithology of the catchment area.

Optical Properties

SPM is a collective term for various groups of suspended material with a broad range of composition, particle size, colour, transparency and refractive index and hence a broad range of optical properties. The **SPM** composition depends upon the local hydrodynamics, the climatic setting and the season. There are to date only few studies publishing specific **SPM** absorption coefficients and backscattering functions (Bukata et al. 1991, Babin 2000, Babin et al. 2003).

Due to the complexity of the **SPM** composition, **SPM** algorithms had always to follow very simplified and generalized concepts. The accepted principle hereby holds that for rising **SPM** concentrations backscattering increases. A commonly used method is to correlate the radiometric signal of a single wavelength band that is minimally influenced by absorption with the **SPM** concentration.

For low to medium **SPM** concentrations the green reflectance maximum is used, such as in Peters et al. (1999), Binding et al. (2003) while the height of the reflectance maximum may be normalized using the NIR such as in Doxaran et al., (2002).

For more turbid waters with higher **SPM** concentration (above 15 mg l⁻¹) the changes of the green reflectance seems to be no more correlated with the **SPM** concentration (Froidefond et al., 2002; Stumpf and Pennock, 1989; Ritchie et al., 1990; Moore et al., 1999). Therefore, for highly turbid waters the applied wavelength range shifts to longer wavelength from the green over the red (Mitchelson-Jacob, 1999; Froidefond et al., 2002) up to the NIR (Dekker 1993).

An early method to detect the most suited wavelength bands for **SPM** estimation in a regional study on eutrophic lakes in the Netherlands was demonstrated by Dekker (1993). For a spectral field data set with corresponding **SPM** concentrations he subdivided the reflectance spectra in 2 nm intervals and calculated correlation between the subsurface irradiance, R , or $R(0-)$, respectively, of these intervals and **SPM**. The resulting wavelength dependent curve (as shown in Fig.3) has its highest values beyond 706 nm with a plateau maximum at 750 nm and a plateau at a slightly lower level in the green to red (600 to 650 nm). Dekker suggested using the 706 band in this case. Although the correlation coefficient is not highest here the strong signal to noise ratio in this wavelength interval surpasses the slightly higher correlation coefficients at 750 nm.

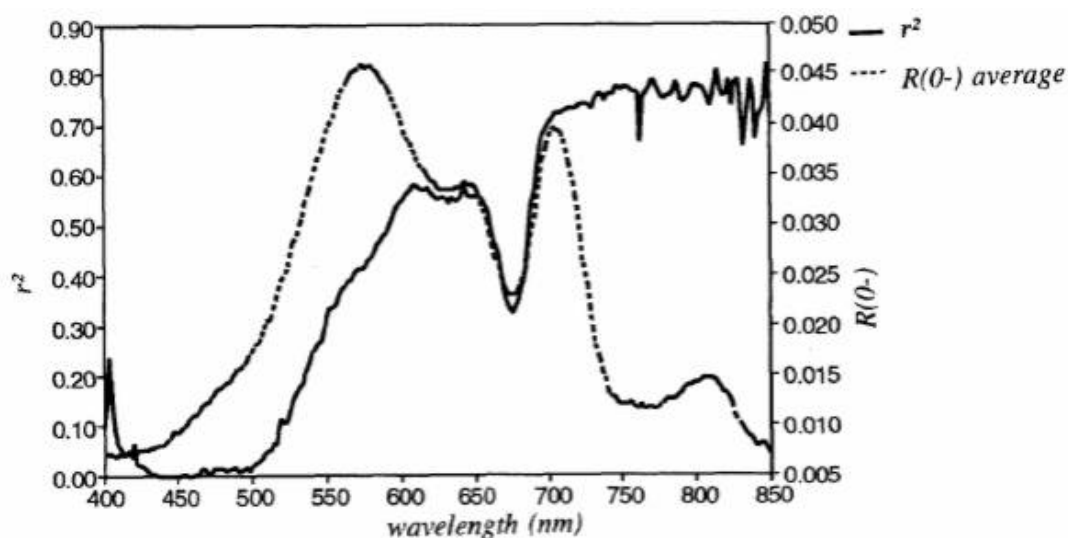


Figure 3: Bivariate linear correlation (r^2) between subsurface irradiance reflectance $R(0-)$ and SPM for 21 samples from Vecht lakes (The Netherlands). The dashed line is the averaged reflectance spectrum of 21 field spectra. The solid line shows correlation between wavelengths (intervals of 2 nm) to corresponding SPM values (Dekker, 1993).

Choice of State of Art Algorithms

The two algorithms described in this report represent widely applied SPM algorithms. Due to the regional and seasonal optical complexity of SPM, both SPM algorithms follow the very simplified concept of the one-band-type algorithm, using both as input parameter the subsurface irradiance, R . This implies that the base of the algorithm performance is an accurate atmospheric correction including the correction for the directly reflected skylight. The operational one band-type SPM algorithm from the Satellite-based Information System

on Coastal Areas and Lakes SISCAL is designed for coastal waters with medium concentrations of predominantly minerogenic SPM, whereas the one band-type SPM algorithm from Dekker (1993) is designed for eutrophic inland waters with high SPM concentrations.

SISCAL Total Suspended Matter Algorithm

Source

Berastegui D., Hansen L. B., Jørgensen, P.V. & Fell, F. (2005): Ocean colour. In Fell, F. (ed.): *Algorithm theoretical basis documents for SISCAL products*.

Jørgensen, P.V (2000). Interpretation of remote sensing ocean colour in Danish coastal waters. *PhD Thesis. Institute of Geography, Univ. Copenhagen, Denmark*.

The algorithm is the operational SPM algorithm of the SISCAL (Satellite-based Information System on Coastal Areas and Lakes) project (<http://www.siscal.net/>) and is based on the work of Jørgensen (2000).

Approach

Based on the principle that rising SPM concentration causes rising reflectance in the visible wavelength range, The SISCAL SPM algorithm uses the green reflectance maximum at 555 nm. Reflectance values of a multi-seasonal field data are correlated by linear regression with SPM concentrations resulting in a linear equation.

Formula

$$SPM = 0,5619 \times R(555) \times 100 + 0,0932$$

Where is:

SPM Suspended Particulate Matter [mg l⁻¹]

R(555) subsurface irradiance reflectance at 555 nm

Input data

Subsurface irradiance reflectance

Field of application

The algorithm was developed for coastal waters of the Danish North Sea where. SPM covers the range from 0,5 to 8 mg l⁻¹ and the subsurface irradiance reflectance values the range between 0,015 and 0,14. The sampled SPM is characterized by a considerable mineral fraction.

Validation

The algorithm has been obtained from an extensive field data set comprising samples from 45 stations taken at all seasons. The algorithm is operationally applied within the SISCAL project.

Acceptance

Accepted

One Band Seston Algorithm by Dekker (1993)

Source

Dekker, A.G. (1993): Detection of optical water quality parameters for eutrophic waters by high resolution remote sensing. *Ph.D. thesis (Vrije Universiteit, Amsterdam, the Netherlands)*.

Approach

The algorithm is based on the principle that rising SPM concentrations cause a proportional increase in backscattering. It takes the reflectance at 706 nm as measure for SPM concentration. The chosen wavelength band at 706 nm represents the best compromise between rising interfering absorption effects (Chl-a absorption feature centred at 675 nm) towards shorter and decreasing signal to noise ratios towards longer wavelength. Reflectance values were correlated to SPM concentrations of a 21 samples comprising field data set by linear regression resulting in a linear equation.

Formula

$$SPM = 2,69 + 331 \times R(706)$$

Where is:

SPM	Suspended Particulate Matter	[mg l ⁻¹]
R(706)	subsurface irradiance reflectance at 706 nm	

Input data

Subsurface irradiance reflectance

Field of application

Highly turbid, productive inland waters. The development of the algorithm is based on a field data set of 21 samples with SPM values ranging from 1 to 45 mg l⁻¹ with a median of 25 mg l⁻¹ from Vecht lakes (The Netherlands).

Validation

The algorithm has been applied numerous times (e.g. Van der Woerd et al. 1999, Koponen et al. 2005) however with different regression coefficients adapted to regional datasets.

Acceptance

Accepted

4.3.4. Coloured Dissolved Organic Matter Algorithms

Coloured Dissolved Organic Matter (cDOM) and Dissolved Organic Carbon (DOC)

Coloured dissolved organic matter (cDOM) also called **Gelbstoff** (Kalle 1949), **yellow substance** or **gilvin**, is one of the major light absorbing constituents in natural waters. This fraction of the **Dissolved Organic Carbon (DOC)** consists of a variable mixture of fulvic and humic acids that stem from degrading phytoplankton and terregineous matter. In general, there is no precise relationship between **DOC** and **cDOM**. However, the practice that is commonly used in the water-processing industry is to relate **cDOM** absorption at a given wavelength to **DOC** concentrations for a given region. Also for given coastal regions specific **cDOM / DOC** relationships can be established (e.g. Ferrari et al., 1996).

The term dissolved is defined operationally, by filtrating the water sample either through a 0.2 µm, 0.45 µm or 0.7 µm pore-size filter. Therefore, measured specific absorption coefficients for **cDOM** have a dependence on the filter pore-size chosen during a specific investigation. Because its absorption is strong in ultraviolet and blue wavelengths, **cDOM** limits the penetration of biologically damaging UV-B radiation but also diminishes available radiation for photosynthesis.

The limnological visual color tests (determination of water colour, ISO, 1994) have been shown to be a good predictor of the absorption by **cDOM** (e.g. Kutser et al., 2005), with regression coefficients between visual colour estimation and **cDOM** absorption varying regionally (Cuthbert and del Giorgio, 1992).

Optical Properties

The absorption of **cDOM** is highest in the UV region and declines to near-zero levels in the red region of the spectrum, causing the yellowish to brownish colours in organic-rich waters. The numerous narrow absorption-bands of this complex organic group cannot be recorded separately by passive optical spectrometric methods. **cDOM absorption (a_{cDOM})** is therefore described by the following exponential equation (Bricaud et al., 1981):

$$a_{cDOM}(\lambda) = a_{cDOM}(\lambda_0)^{-S(\lambda-\lambda_0)} \quad [\text{m}^{-1}]$$

The exponential Slope gradient, S , generally lies between 0,01 to 0,02 nm⁻¹ (Babin et al., 2003). The most common means of expressing its concentration is through the use of the specific absorption coefficient at some reference wavelength, typically $a_{cDOM}(254)$, $a_{cDOM}(400)$, $a_{cDOM}(410)$, $a_{cDOM}(440)$. They can also be termed Specific Absorption Coefficients: SAC254, SAC400, SAC410, SAC440.

cDOM algorithms have been mainly derived from ship borne spectroradiometer measurements (Hirtle and Rencz, 2003; Kutser et al., 1998) or using an airborne spectrometer (Kallio et al., 2001). Because the absorption by **cDOM** decreases exponentially with increasing wavelength, the influence on the remotely sensed signal is strongest in the blue wavelength range. However, high **cDOM** concentrations result in low water-leaving reflectance close to zero and therefore require highest radiometric sensitivity in the blue wavelength range. Atmospheric correction of blue wavelengths is challenging, especially in the case of strongly absorbing waters with low reflectance. Just as the determination of Chl-a using remote sensing algorithms is compromised by the presence of **cDOM**, so the

determination of **cDOM** absorption in the blue wavelength region will be sensitive to high concentrations of Chl-a.

Therefore, the information in the longer wavelength region is preferred for algorithm development, often normalized with a red wavelength-band (outside of the spectral influence of **cDOM**) such as in the approaches of Kutser et al. (2005) and Schwarz (2001). A potential way to improve remote sensing **cDOM** algorithms could be an application of colour classification and then optimization of the algorithms for specific classes (e.g. Darecki et al. 2003, Lahet et al. 2001).

Choice of State of Art Algorithms

Three algorithms are described in this report: The cDOM algorithm by Kutser et al. (2005) is designed for organic-rich inland waters. The cDOM algorithm by Kowalczyk et al. (2005) performs in organic-rich coastal waters. The DOC algorithm by Schwarz (2005) can be merged with the cDOM algorithm by Kowalczyk et al. (2005) or runs separately.

Lake cDOM Band Ratio Algorithm by Kutser et al. (2005)

Source

The band-ratio type cDOM algorithm was developed using atmospherically corrected Advanced Land Imager (ALI) data and a large field campaign with $a_{cDOM}(420)$ field measurements in organic-rich boreal lakes in Finland and Sweden. The algorithm and detailed evaluation is described in:

Kutser, T., Piersona, D.C., Kallio, K.Y., Reinart, A. & Sobek, S. (2005). Mapping lake cDOM by satellite remote sensing. *Remote Sensing Environm.*, 94, 535–540.

Approach

Absorption by cDOM decreases exponentially with increasing wavelength. Theoretically, the influence of cDOM on the remotely sensed signal in ALI band 1 (450–515 nm) is stronger than in band 2 (525–605 nm). However, there are several reasons why Kutser et al. (2005) chose band 2 (B2). Atmospheric correction of blue wavelengths (band 1) is often a problem, especially in the case of strongly absorbing waters with low reflectance. At the same time sensitivity of blue sensors is often inadequate. Therefore, the ALI band2/band3 ratio has proven to be more suitable for cDOM retrieval (correlation: $r^2=0,73$). ALI band 3 (630–690 nm) is used for normalizing purposes as the influence of cDOM in B3 (630–690 nm) is practically negligible. The relationship of the band ratio values can be described with a power function.

Formula

$$a_{cDOM}(420) = 5.13 \left(\frac{R_s(525,605)}{R_s(630,690)} \right)^{-2.67}$$

Where is:

$a_{cDOM}(420 \text{ nm})$	cDOM absorption at 420 nm [m ⁻¹]
$R_s(525,605)$	surface reflectance at 525 to 605 nm (respectively at 630 nm to 690 nm)

Input Data

Surface reflectance

Field of application

The algorithm is based on 2 atmospherically corrected ALI acquisitions and a large field data set in organic-rich boreal lakes in southern Finland and Sweden. In situ measurements were carried out in 34 lakes (39 stations). The study areas covered a large variety of lake sizes with variable cDOM concentrations:

$a_{\text{cDOM}}(420)$ varied between 0.68 and 11.13 m^{-1} . Kutser et al. (2005) state that the cDOM retrieval algorithm is valid for a wide variety of optically different lakes in different geographic locations and can be used operationally for space borne mapping of cDOM in lakes. The concentration of cDOM in boreal lakes is in correlation with DOC (Tranvik, 1990).

Validation

The algorithm was validated using data of an additional ALI and field campaign. The water-colour data (routinely collected by the Finnish Environment Institute) were converted towards $a_{\text{cDOM}}(420)$. The $a_{\text{cDOM}}(420)$ values estimated from the evaluation data set were well correlated with in situ data ($r^2=0.83$).

Acceptance

Accepted

Coastal cDOM Log Band Ratio Algorithm by Kowalczyk et al. (2005)**Source**

Kowalczyk, P., Olszewski, J., Darecki, M. & Kaczmarek, S. (2005). Empirical relationships between coloured dissolved organic matter (cDOM) absorption and apparent optical properties in Baltic Sea waters. *Int. J. Remote Sens.*, 26(2), 345–370.

This paper summarizes results of a large, multi-temporal and multi-seasonal data set from 39 cruises between 1993 and 2001 in the southern organic-rich Baltic Sea.

Approach

The seasonal change of ship borne reflectance values compared to laboratory cDOM(440) measurements obtained at 39 Baltic Sea cruises from 1999 to 2001 were investigated with the following important consequences for cDOM remote sensing:

- i) Very small reflectance values at 412 nm and virtually no temporal and spatial variations excluded the short blue wavelength range.
- ii) The 440 nm wavelength is affected by the absorption of phytoplankton pigments and is therefore excluded.
- iii) The 490 nm wavelength was chosen because it is separated from the main phytoplankton absorption peak and cDOM absorption at this wavelength is still significant in organic-rich coastal waters.

The 590 nm wavelength was chosen as reference band based on the work of Darecki et al. (2003). These findings have been adopted to examine the empirical relationship between

cDOM(400 nm) absorption and a band ratio of 490 and 590 nm on a log scale (n=599). The best approximation of the whole data set is presented by a second-order polynomial.

Formula

$$a_{cDOM}(400nm) = 10^{-0,2-0,5[R_{rs}(490)/R_{rs}(590)]+0,65[R_{rs}(490)/R_{rs}(590)]^2}$$

Where is:

$a_{cDOM}(400)$	absorption of cDOM at 400 nm	$[m^{-1}]$
$R_{rs}(490)$	remote sensing reflectance at 490 nm (respectively at 590 nm)	$[sr^{-1}]$

Input Data

Remote sensing reflectance

Field of application

The algorithm was developed for the case 2 waters of the Baltic Sea. Because of its semi-enclosed character and very high organic-rich terrigenous input by rivers, the Baltic Sea has unique optical properties dominated by cDOM (e.g., Jerlov, 1953).

The presented cDOM algorithm is based on the qualitative and quantitative statistical analysis of the impact of cDOM absorption on the spectral reflectance in the southern part of the Baltic Sea. The bio-optical data were collected by researchers of the Institute of Oceanology, Polish Academy of Sciences, Sopot, Poland, over an eight-year period (1993–2001). The algorithm may be transferable onto similar coastal waters influenced by organic-rich freshwater input, such as Arctic coastal seas.

Validation

Regression analysis showed a systematic error of 4 % and a random error of 32 %. The algorithm overestimates low cDOM(400) absorption values and slightly underestimates high cDOM(400) absorption values. The algorithm gives the best satisfactory estimation for intermediate cDOM(400) absorption values (0.5 to 2.0 m^{-1}).

Acceptance

Accepted

Baltic Sea DOC Algorithm by Schwarz (2005)

Source

Schwarz, J.N. (2005). Derivation of dissolved organic carbon concentrations from SeaWiFS data. *Int. J. Remote Sens.*, 26(2), 283–293.

The organic-rich Baltic Sea was chosen as ideal test site for remotely sensed DOC. DOC is calculated from cDOM that is derived by a band-ratio type algorithm.

Approach

1) derivation of cDOM

In the first step, a band ratio type algorithm with wavelengths at 443 nm and 512 nm by Schwarz (2001) is used to estimate $a_{cDOM}(440)$.

2) derivation of DOC

In a second step, DOC is calculated from cDOM with established regional conversion factors. The DOC algorithm by Ferrari et al. (1996) was chosen by Schwarz (2005) as being the most representative algorithm for the Baltic Sea. First, values of $a_{cDOM}(440)$ have to be converted to $a_{cDOM}(335)$ taking the value for S of 0.019 nm^{-1} . S is known to take a broad range of values, however, for the Baltic, Schwarz et al. (2002) reported a specific S value of $0.0193 \pm 0.0024 \text{ nm}^{-1}$.

Formula

- 1) $\ln a_{cDOM}(440) = -0.1123 - 0.8725 \ln \frac{R_{rs}(443)}{R_{rs}(512)}$
- 2) $S = 0.019; a_{cDOM}(335) = a_{cDOM}(440)^{-0.019 \times (335 - 440)}$
- 3) $DOC = 3.39(\pm 0.217) + 0.589(\pm 0.109)a_{cDOM}(335)$

Where is:

$a_{cDOM}(440)$	cDOM absorption at 440 nm, respectively at 335 nm	$[\text{m}^{-1}]$
DOC	Dissolved Organic Carbon	$[\text{mg l}^{-1}]$
R_{rs443}	remote sensing reflectance at 443 nm (respectively at 512 nm)	$[\text{sr}^{-1}]$
S	Slope of the semi-logarithmic absorption spectrum	$[\text{nm}^{-1}]$

Input Data

Remote sensing reflectance

Field of application

The algorithm was developed for the case 2 waters of the Baltic Sea. Because of its semi-enclosed character and very high organic-rich terrigenous input by rivers, the Baltic Sea has unique optical properties dominated by cDOM (e.g., Jerlov, 1953).

The cDOM algorithm by Schwarz (2005) is based on 24 data sets of in-water spectroradiometrical measurements and $a_{cDOM}(440)$ measurements from a Baltic Sea cruise in 1997. The cDOM / DOC conversion factors for the Baltic Sea were chosen by Schwarz (2005) employing an intensive literature study and expert communications. Ferrari et al. (1996) from whom the DOC algorithm is taken, measured in the range of 5.22 mg l^{-1} to 7.39 mg l^{-1} in the southern Baltic Sea.

The DOC algorithm may be transferable onto similar coastal waters influenced by organic-rich freshwater input, such as Arctic coastal seas.

Validation

Regression analysis showed an error of 50% in Schwarz (2001). Schwarz (2005) emphasizes also to use alternative cDOM algorithms from multiannual data sets such as the cDOM algorithm by Kowalczyk et al. (2005) (*this report*). This study accounts for a 9-year data set in the Baltic Sea, unique in spanning a enormous range of variability in all parameters, and thereby reducing the statistical uncertainty in the cDOM retrieval technique.

The uncertainty in S has a standard deviation in of 12.6 %. Reported uncertainties (Ferrari et al., 1996) for formula 3) are the standard deviations in DOC intercept of 6.4 %, and in DOC slope of 18.5 %. Schwarz (2005) discusses that the highest contribution to error in DOC estimates comes from the large uncertainty in the DOC slope and that greater confidence in the estimation of DOC concentrations will only follow from an increase in in-situ investigations sampling of DOC and cDOM absorption together.

Acceptance

Accepted

4.4. Forward and Inverse Hyperspectral Modelling

Choice of State of Art Algorithms

There are several established approaches using the numerical approximation of an hyperspectral hydro-optical model. Long-term practical experience, successively refined models, long-term validation of products and a highly international scientific reputation are provided by the choice of expert groups that we have contacted and that we additionally propose.

Following expert groups have been contacted:

1. Earth Observation and Mapping EOMAP GmbH & Co.KG, Gilching, Germany
contact person: Dr. Thomas Heege
2. GKSS-Forschungszentrum Geesthacht, Geesthacht, Germany
contact person: Prof. Roland Dörffer
3. NIERSC, St. Petersburg, Russia
contact person: Prof. Pozdnyakov

Following expert groups are further recommended:

4. German Space Agency, Deutsches Zentrum für Luft- und Raumfahrt (DLR),
Berlin-Adlershof, Germany
phone: +49-(0)30 67055-640
fax: +49-(0)30 67055-642
Contact person: Dr. A. Neumann, email: andreas.neumann@dlr.de
5. Free University of Berlin, Freie Universität Berlin (FUB), Institute for Space Sciences,
Berlin, Germany
phone: +49-(0)30-838 56 666
fax: +49-(0)30-838 56 664
Contact person: Prof. J. Fischer, email: juergen.fischer@wew.fu-berlin.de

4.4.1. EOMAP, Gilching, Germany

EOMAP GmbH & Co.KG, <http://www.eomap.de>
Sonderflughafen Oberpfaffenhofen, Geb. 319
Friedrichshafener Str. 4a
82205 Gilching, Germany
phone: +49 (0)8153 - 9875 40
fax: +49 (0)8153 - 9875 55
Contact person: Dr. Thomas Heege, email: heege@eomap.de

Approach

Inversion data processor is the Modular Inversion Program (MIP) that is developed for applications in inland and coastal waters. The hyperspectral services include:

atmospheric correction, aerosol concentrations, sun glint and glitter and sky glint correction

Chl-a, SPM, cDOM

bathymetric mapping, macrophyte mapping, sea floor mapping

4.4.2. GKSS, Geesthacht, Germany

GKSS Forschungszentrum Geesthacht
Max-Planck-Straße 1
21502 Geesthacht, Germany
phone: +49 (0)4152 87-158
Contact person: Prof. Roland Dörffer, email: roland.Dorffer@gkss.de

Approach

Inversion data processor is the *Regional Case 2 processor (C2R)* that is developed for applications in coastal waters. The hyperspectral services include:

atmospheric correction, aerosol concentrations, sun glint and glitter and sky glint correction

Chl-a, SPM, cDOM, Secchi depth

GKSS needs one man/year to design a plug-in tool for the hyperspectral Enmap tool box.

4.4.3. NIERSC, St. Petersburg, Russia

Nansen International Environmental and Remote Sensing Center **NIERSC**
a Non-Profit/ Project-Oriented International Research Institute for Environmental and Climate Study founded in 1992 in St. Petersburg
Vasilievsky Island 14th Line, 7A,
199034 cSt. Petersburg, Russia
Phone: +7 (812) 324-51-03,
Fax: +7 (812) 324-51-02
Contact person: Prof. Pozdnyakov, email: dmitry.pozdnyakov@niersc.spb.ru,

Approach

The algorithm is based on the Levenberg-Marquardt multivariate optimization procedure starting with the atmospherically corrected reflectances and can be merged with the atmospheric correction of the *Regional Case 2 processor C2R (GKSS)*. Applications have

been designed and evaluated for Russian Arctic coastal waters. The hyperspectral services include:

Chl-a, SPM, DOC

NIERSC cannot provide the source files of the programs that realize the algorithm but can provide the respective binary executable files. The programs are written in Matlab, but can be rewritten in C++, or Java, or IDL.

5. Review of Algorithms and Products with Relevance for the EnMAP Toolbox Issue – Man Made Surfaces

Wieke Heldens, Enrico Stein and Andreas Müller



5.1. Introduction

This study provides a review of algorithms and products with relevance for EnMAP with a focus on man made surfaces. Man made surfaces in this study are defined as artificial surfaces (e.g. asphalt, concrete, (synthetic) roofing materials) representing the main land cover of human settlements and transportation networks. Reservoirs, mining waste dumps and similar objects created by humans are not considered as man made surfaces. Remote sensing for mining landscapes is discussed in the section on geology. The focus of this review on algorithms and methods relevant for the EnMAP toolbox for man made surfaces will be on urban areas. An analysis of the state of the art in hyperspectral applications for man made surfaces is provided. As case studies of hyperspectral applications in urban environments are scarce, additionally a summary on typical application fields for classical remote sensing techniques in this field is presented. Both sections then are used as a basis for deriving recommendations and requirements for using EnMAP in urban studies.

Mapping of urban areas provides scientists and urban planners with up-to-date information on urban land cover and land use. Monitoring and analysis of urban growth is also an important topic, especially in rapidly growing cities, where urban sprawl is a large problem. The acquired information can be used in scenario studies for the development of the city, for environmental studies, e.g. on the living quality for the inhabitants

To fulfil those information needs remote sensing in general is an accepted tool. Using aerial imagery for mapping, e.g. for producing topographic maps or cadastres is common. It used to be very time consuming, because the images were mainly manually interpreted. Recently, more (automatic) approaches are up-coming and are constantly improved towards operational usage. The main use of remote sensing for urban analysis is still scientific, because of the high costs of data acquisition and the need of remote sensing experts to process the data. The most important application fields of remote sensing for urban analysis are urban land cover /land use mapping, urban planning, monitoring of urban growth, risk analysis and urban climate.

Certain aspects have to be taken into account when remote sensing is used for urban analysis. Man made surfaces, especially when they occur in urban areas are characterised by many materials and objects varying over short distances, resulting in a heterogeneous surface cover. In comparison to 'natural' areas, the borders between the different land covers are crisp. This makes the urban area into a complex environment. From an optical remote sensing point of view this leads to clearly separable spectra and objects if the spectral and spatial resolutions are high enough. With lower spatial resolutions many mixed pixels occur, because there are multiple objects within one pixel. Lower spectral resolutions cause small characteristic features to become invisible and reduce the variability between the spectra of different materials. This is a difficulty, since many sensors do not meet the optimal requirements. Therefore in many studies approaches have been developed to deal with lower spatial and / or spectral resolution while mapping relevant urban parameters.

When summarizing the methods of scientific publications on this subject, four trends in urban remote sensing can be recognised.

The first trend is the usage of medium resolution data (i.e. 30x30 m²), which is easily available. The studies mainly focus on land cover in general classes, for example for mapping urban growth or analysing the relation between the city and its surroundings.

The second trend uses very high resolution imagery. Since with such sensors not so much spectral information is available, mostly only three or four broad bands, the spatial and texture information is used intensively. This is often applied for mapping urban structure, buildings or roads with high detail, since spatial resolutions of 1 meter and less are available.

The third trend that can be recognised, though not as common as the other two, is the use of hyperspectral sensors. Because most of those sensors are airborne, their spatial resolution is quite detailed, between 2.5 and 15 meter. In studies following this trend the main questions are about mapping and identifying man made materials and urban vegetation.

A fourth trend, becoming more and more popular, is a combination of the above trends. High resolution imagery, including digital surface models, expands the information content of lower resolution imagery. It allows making use of the full spectral information of the multispectral or even hyperspectral images and, at the same time, takes advantage of the spatial detail of high spatial resolution imagery.

With EnMAP, being designed as a hyperspectral satellite based sensor with medium spatial resolution, a new category of imagery will become available, providing interesting opportunities for analysis of man made materials and urban area. In the following review, the state of the art of hyperspectral remote sensing of man made surfaces is provided and an overview is given of existing methods for mapping the most important parameters for analysis of man made surfaces. Based on this, recommendations are made on how the potential of EnMAP can be used for urban area mapping. Methods and algorithms that are suitable for the EnMAP Toolbox are described as well as research activities are recommended to improve existing methods for the EnMAP data.

5.2. Main Topics in Hyperspectral Remote Sensing Applications and Man Made Surfaces

Since hyperspectral remote sensing is not widely available yet, many of those application fields are covered by multispectral remote sensing. In this chapter, first the state of the art of hyperspectral remote sensing for urban analysis is presented. Secondly, the main application fields of urban remote sensing are described.

5.2.1. State of the Art in Hyperspectral Applications for Man Made Surfaces

Since the nineties hyperspectral remote sensing started to be used for urban studies. Though hyperspectral remote sensing is still mainly experimental, large potential has been identified for its use for urban analysis. Small (2001) showed with use of MNF transformations that the spectral dimensionality of urban areas is up to 2.5 times higher than that of non-urban areas. To cover this spectral dimensionality, a hyperspectral sensor recording also small characterising features is required. Herold et al. (2004) show in a

comparison of IKONOS, Landsat and AVIRIS data that the hyperspectral sensor AVIRIS retrieves the best classification results, especially when aiming at identifying different roof materials. Small (2001) and Herold et al. (2003) also take the spatial resolution into account. The average size of urban objects is 10-20 meter, making the choice for sensors with a high spatial resolution for urban analysis fairly logic. With lower spatial resolution the amount of mixed pixels increases. However, a study of Cavalli et al. (2008) shows that a classification of the urban area of Venice, Italy with the hyperspectral sensor Hyperion (30 x 30 m² pixel size) has similar accuracy as classification results of the higher resolution multispectral sensor MIVIS (8 x 8 m² pixel size). Because of the high spectral resolution hyperspectral data has much more potential for analysing mixed pixels than multispectral data. Especially in urban areas this is a large advantage. Hyperspectral data is therefore used more and more. Because of the lack of suitable satellite based hyperspectral sensors for urban areas, most studies have been carried out with airborne hyperspectral sensors. Depending on the subject of the study different methods and additional data are used.

Analysis of the spectral characteristics of man made surfaces is often carried out by field spectroscopy or high resolution airborne hyperspectral data in combination with field spectroscopy. Using different spectral analysis techniques man made materials are characterised (e.g. Bassani et al. 2007; Heiden et al. 2007). Several aspects influence the spectra of man made materials. The effects of aging on the man made materials are an important research topic. Usage, dust and erosion can largely change the spectral signature, e.g. for asphalt as described by Herold and Roberts (2005). Also BRDF effects can become quite large in urban areas. Roofs are differently illuminated because of their slope and orientation. Shadows are cast by the large number of buildings. This reduces the albedo of the spectra in the shadow or even makes them unrecognisable because of the sensor noise with existing space borne and many airborne sensors (Lacherade et al. 2005). Richter and Müller (2005) developed an algorithm to de-shadow spectral imagery. The algorithm corrects spectra for shadows cast by clouds and buildings. This makes it possible to recognise the spectral characteristics again. Knowledge on the spectral characteristics of the man made materials is used to identify them in hyperspectral images, using a large variety of methods

Information on the available spectral characteristics is used for selecting the methods and classes for mapping urban land cover. Based on the selected method and used data set, the classes are selected differently. Usually 'standard' land cover classes such as 'soil', 'water' and 'vegetation' are included. Depending on the focus of the study and the quality of the spectra in the study area, the detail of the mapped classes can be up to single roof and street cover materials (e.g. Heiden et al. 2007). In section 0 the issue of classification schemes is addressed in more detail.

Because of the relatively small objects in urban areas and the resulting high amount of mixed pixels, spectral unmixing approaches are used frequently (e.g. Ben-Dor et al. 2001; Segl et al. 2003). Also spectral angle mapper (SAM), a method to classify pixels by comparing image spectra with known endmember spectra is often used (e.g. Bhaskaran et al. 2004; Chen and Hepner 2001). Of course more traditional classification approaches are applied as well, both on original bands as on transformed spectral bands, such as maximum likelihood classification (e.g. Dell'Acqua et al. 2005; Herold et al. 2004). A transformation of spectral bands is applied to reduce the noise, correlated bands or data dimensionality, for example

with a MNF (minimal noise fraction) transformation or principal component transformation. A few research groups work on extensive mathematical approaches such as morphological profiles to analyse urban hyperspectral data (Benediktsson et al. 2004; Plaza et al. 2004). In those approaches also the spatial organisation is taken explicitly into account. Spatial information can provide very useful a priori information for the classification of urban areas. Because the borders of urban objects are usually crisp, image segmentation is a promising approach, which gains more and more attention, also for hyperspectral data. An interesting example is the use of support vector machines (SVM) to model and classify at segment level (e.g. Lizarazo 2008; van der Linden et al. 2007).

Frequently a combination of data sets is used for the classification of urban areas. Often the hyperspectral data is extended with information from other sources. A common aim of using such additional data is to identify buildings a priori to the classification. Various data sources are used such as a digital elevation model (DEM) derived by stereo imagery (e.g. Greiwe et al. 2004; Madhok and Landgrebe 1999), cadastre data. (e.g. (Heldens et al. 2008) or lidar or radar data (e.g. Bochow et al. 2007; Chen et al. 2003). Very high resolution imagery is used as well in combination with hyperspectral data, at different levels of data fusion (e.g. Gamba et al. 2007; Niemann et al. 1998).

5.2.2. Typical Application Fields for Remote Sensing of Man Made Surfaces

In this section the most important application fields for urban remote sensing are described. Using remote sensing for urban analysis is a suitable way for acquiring information when cadastre or topographical maps are unreliable, out of date or do not exist. Remote sensing data are usually more efficient in time and money than mapping the area by field work, especially when full area coverage is needed. Additionally, information that easily can be retrieved from remote sensing data might be difficult to obtain by field surveys. Those aspects make urban analysis with use of remote sensing of interest for both developed and undeveloped countries.

Urban Land Cover /Land Use Mapping

Urban land cover and land use can be mapped at different scale levels. With remote sensing only the land cover can be assessed. Some studies map land use indirectly by linking land use classes to land cover classes (e.g. Lu and Weng 2006). The selected classification scheme depends on the observation scale. In many studies a hierarchical classification scheme is used (e.g. Herold et al. 2004; Roessner et al. 2001). Probably the best known scheme is the land cover /land use classification scheme of Anderson et al. (1976). This scheme has been developed for the Geological Survey in the U.S. and consists of four levels. Level I contains the main land cover classes, such as vegetation, water, built up/artificial surfaces, water and bare soil. In level II the classes of level I are subdivided according to their function or other generic characteristics. Level III and IV are user defined classes. In urban studies those levels contain for example man made materials, which are separated after their material properties and spectral characteristics. An example of how the Anderson scheme can be applied for urban analysis is provided in Table 1. An additional hierarchical classification scheme for urban areas is presented in Figure 2.

Table 1: Anderson classification scheme adapted for urban analysis (after Herold et al. 2004)

Level 1	Level 2	Level 3	Level 4
Built up	Buildings/Roofs	Composite shingle roof	Black shingle
			Blue shingle
			Brown shingle
			(...)
		Plastic roofs	
		Glass	
		Gravel roof	Gray gravel
			Red gravel
		Metal roof	Brown metal
			Light grey metal
			Green Metal
		Asphalt roof	Light grey asphalt
		Tile roof	Red tile
			Grey tile
		Tar roof	Black tar
			Brown tar
		Wood shingle roof	Dark wood shingle
	Transportation areas	Asphalt roads	Light asphalt (old)
			Dark asphalt (new)
		Concrete roads	Light concrete
		(...)	
	Sport infrastructure	Tennis courts	
		Red tartan	
		Basketball court	
Vegetation	Green vegetation		
	Non-photosynthetic vegetation		
Non-urban surfaces	Bare soil		
	Beach		
	Bare rock		
Water bodies	Natural/quasi-natural bodies		
	Swimming pools		

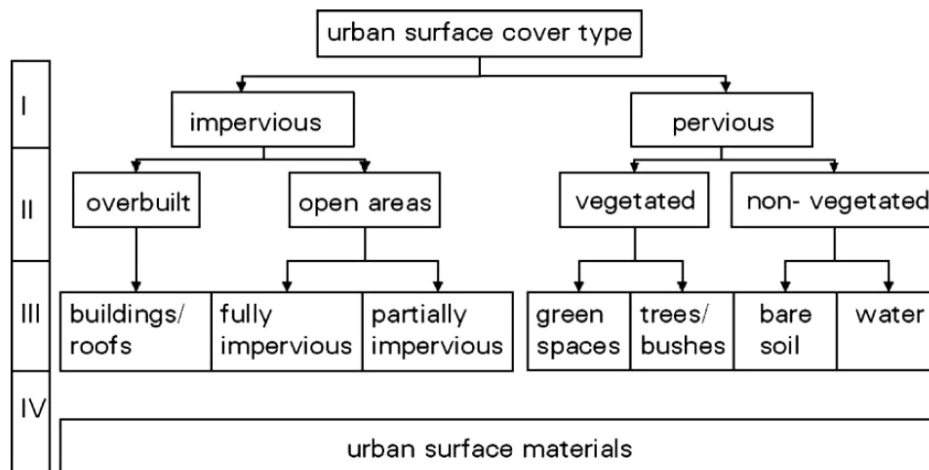


Figure 2: Hierarchical urban classification scheme for urban biotope mapping (Heiden et al. 2007)

Not always the classification schemes are that systematically defined. Often several classes at the highest hierarchical level are selected, extended with several spectrally distinct classes or classes that are of special interest for the study. The classification methods that are used for mapping urban land cover are numerous. For urban land cover classifications the same methods are used as for other land cover classifications. Spectral unmixing approaches and support vector machines are popular. An overview of the most common different urban land cover classification methods is presented in Table 2.

Table 2: Overview of common urban land cover mapping methods

Method	Remarks	applied in (amongst others):
Linear Spectral Mixture Analysis (LSMA)	Provides a solution for mixed pixels. Depending on the approach, different numbers and combinations of EM are allowed to model the mixed spectrum (e.g. MESMA). Provides the abundance of a material/class within a pixel.	(Bochow et al. 2007; Chen and Li 2008; Lee and Lathrop 2005; Lu and Weng 2006; Pu et al. 2008; Roessner et al. 2001; Small 2003)
Support Vector Machines (SVM)	The image to classify can contain other data than only spectral information (e.g. height, geometric info, etc). Often applied on or in combination with image segments	(Bruzzone and Carlin 2006; Inglada 2007; Lizarazo 2008; van der Linden et al. 2007)
Spectral Angle Mapper (SAM)	Insensitive to differences in albedo, takes the shape of the complete spectrum into account. Especially suitable for hyperspectral data	(Bhaskaran et al. 2004; Chen and Hepner 2001; van der Meer 2006)
traditional supervised classifiers	Maximum likelihood, minimum distance, parallel-piped, etc; For hyperspectral data often a data reduction is needed	(Gluch et al. 2006; Madhavan et al. 2001)
Neural Networks	No particular distribution of the data assumed. The trained classifier is a black box	(Berberoglu et al. 2000; Song et al. 2005)

A common approach in urban land cover mapping is image segmentation, applied before or during the classification. Especially for imagery with high spatial resolution, this procedure is often applied. Since in urban areas the borders between the objects are very crisp, the image segmentation algorithms are usually quite successful and represent the urban objects quite

well. This improves the subsequent, object oriented classification. Rule based classification (e.g. as implemented in the image segmentation software DEFINIENS (Batz and Schäpe 1999) (e.g. Banzhaf 2007) is one popular method for classifying image segments in urban land cover studies. But since the use object oriented classification is increasing rapidly for urban studies, many classification methods for image segments are tested, such as classification with Support Vector Machines (e.g. Lizarazo 2008; van der Linden et al. 2007) or Spectral Angle Mapper (e.g. Cavalli et al. 2008; Greiwe et al. 2004).

Material mapping

Material mapping is another way to describe the urban surface. It requires a different perspective than for land cover mapping. Similar materials can be found on different land cover types. Hydrocarbons, for example, can be used on roofs (tar) and roads (asphalt) (Herold et al. 2007). For material mapping mainly hyperspectral data is used. Only such data provides enough spectral information to separate the materials by their spectral characteristics. The spectral signatures are defined by the chemical composition of the man made materials. For example in many synthetic materials such as polyethylene and bitumen, hydrocarbons (CH-chains) are present. All spectra of such materials have more or less present adsorption features starting at $2.2\mu\text{m}$ and continuing towards longer wavelengths, caused by the CH-chains (Heiden et al. 2007). Depending on the objective of the study, only one material is looked for (target detection) or the whole area is mapped. The materials can be identified by their spectrum, following similar principles and methods used in geology to identify minerals, i.e. using position, depth and width of adsorption features.

A common method is to compare image spectra to endmembers, spectra of known materials. There are many ways to do that. Both classifiers which assign one class to each pixel and spectral unmixing approaches assigning more than one class to each pixel are used. Many measures exist to evaluate the similarity of an unknown spectrum to a known endmember spectrum. Spectral Angle Mapper (SAM) (e.g. used in Chen and Heppner (2001) is only one example; other examples are Euclidian minimum distance (ED) or spectral information divergence (SID), for example used in Chen et al. (2008). Van der Meer (2006) compares four spectral similarity measures (SAM, ED, SID and spectral correlation measure (SCM)) in their ability of separating four mineral spectra. The different measures vary in their sensitivity to noise and the selected spectral region. SID turned out to be more effective in mapping the four selected minerals, SAM and ED reach similar results.

Spectral unmixing is especially suitable in urban areas, because even with quite high spatial resolution (4-10 m) many mixed pixels occur. Roessner et al. (2001) developed an unmixing approach especially for identifying urban materials. Based on characteristic features, endmembers are selected from the image. In the next step the spectral unmixing is carried out, mapping the cover fraction of all materials. Ben Dor et al. (2001) used a partial unmixing analysis. This Mixed Tuned Matched Filtering (MTMF) approach maximises the response of known endmembers and suppresses background signals. Also for this study extensive spectral endmember libraries have been collected, since the variation of materials in urban areas is very large.

V-I-S Concept

Next to the hierarchical classification scheme another concept is often applied for mapping urban land cover. This is the vegetation-impervious-soil (VIS) model, developed by Ridd (1995). This concept is often used for analysis at medium scales, comparable with the scale of Andersons Level I. According to this concept, urban area can be modelled by vegetation, impervious surface (buildings, streets etc.) and soil (see Figure 3). Those three parameters are important because they support analyses of the physical aspects of urban area, such as land cover changes and the urban heat island phenomenon on the one hand. On the other hand analysis of the social aspects of urban environments, such as population density and socio-economic development level is supported. The three model components are very suitable to be mapped by remote sensing, because they have different spectral characteristics. Vegetation, impervious surface and soil can be considered as three endmembers in an unmixing model. In an urban area those three components occur next to each other within meters. Linear spectral unmixing is therefore a very common method to map urban area according to the V-I-S concept. Among others Powel et al. (2007) and Pu et al. (2008) used a spectral unmixing approach. To improve the quality of the endmembers in several studies the impervious class is replaced by high albedo and low albedo endmembers (e.g. Chen and Li 2008; Lu and Weng 2007). The disadvantage is that the low albedo endmember also includes water and shadow and thus not only impervious surfaces. All studies mentioned above noticed that with multispectral data, it is difficult to identify imperviousness and separate it from soil. Using hyperspectral data or reference endmember additional to image endmember could improve the identification of impervious surface (Lu and Weng 2007).

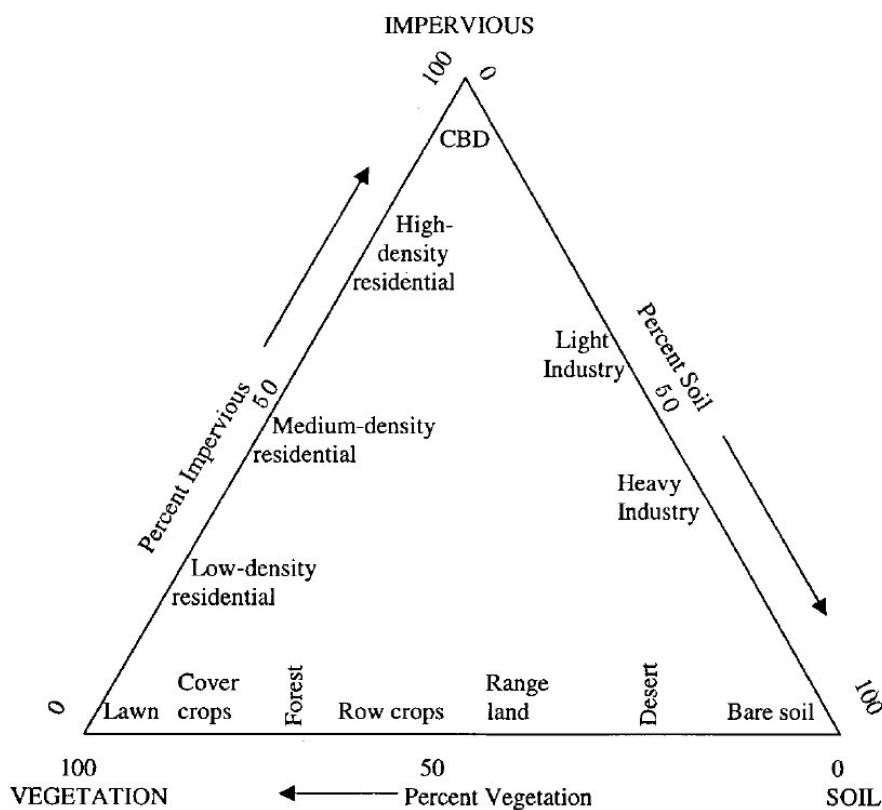


Figure 3: V-I-S Concept after Ridd (1995)

Urban Planning

A clear definition of urban planning is hard to find. Generally the activities of governments concerning the planning of development and improvement of urban areas are meant. This can include zoning, design of single blocks and neighbourhoods or more abstract directives at city or regional scale. Depending on the organisation that is carrying out the planning activity, the emphasis can differ: architecture, traffic, ecology, sustainability etc. To design rational plans, many aspects should be taken into account. Causes for unwanted developments need to be identified and alternatives offered. Of course therefore information is needed about the location and growth of the city. But also knowledge is required on the number and expected growth of inhabitants, the quality of the living areas and the availability of facilities like shops, schools and hospitals, to name just a few parameters. The possibility to map complete urban areas fast and frequently caused many researchers to use remote sensing data for urban planning. Frequently, an urban land cover classification provides useful information on the general organisation of the urban area (see section 0 for common methods).

Imperviousness

Imperviousness is a key parameter for urban analysis (Lu and Weng 2006) and very important for urban planning. Imperviousness can be mapped by aggregating all classes of a land cover classification which completely seal the surface, such as buildings and asphalt. In land cover classifications according to the V-I-S concept imperviousness is already a separate class. Since this class is spectrally not so clearly to separate, Wu and Murray (2003) presented a method to improve the mapping of impervious surface. With spectral unmixing analysis they estimate the fractions of the four endmembers vegetation, soil, high and low albedo from Landsat data. They state that impervious surface cannot be an endmember due to its large variability. Impervious surfaces are likely to be located on or near to the line connecting the high and low albedo endmembers in the feature space. After masking out the non-impervious surfaces (e.g. water, clouds and sand) from the high and low albedo fractions in the unmixing result, the imperviousness can be calculated for each pixel by adding the high and low albedo abundances. The accuracy assessment of the study shows an overall estimation RMS error of 10.6% for the calculated impervious surface fractions. The method presented by Wu and Murray (2003) is implemented in several other studies, for example in Weng et al. (2008) and Lu and Weng (2006). The latter combined the impervious surface fraction with population numbers to characterise urban land use. A low-intensity residential area for example, is characterised by little impervious surface and a population density of less than 500 persons / km².

Another approach of mapping impervious surface is developed by Esch et al. (2008). In this study is the estimation of impervious surface based on Landsat images using a Support Vector Machine. The training of the classifier is automated and is based on impervious maps derived from high spatial resolution data or from a vector data set e.g. from the cadastre. With this tool the imperviousness of the complete German state of Bavaria has been calculated. This can support the government in monitoring their results in their aim to reduce the daily increase of impervious surface.

Buildings and Built up area

Identification of buildings is often important. Unfortunately it is not that straight forward with optical remote sensing, since building roofs consists of many different materials; there is not one building spectrum. Therefore in many studies the class 'buildings' is divided in several classes according their spectral characteristics (for example red, grey and white roofs (Bruzzone and Carlin 2006)). At scales larger than single houses often the classes high and low building density are used, e.g. in Song et al. (2005). Because of the increase of vegetation and soil between the buildings in area with lower building density, the spectrum (which actually consists of a mixture of impervious materials, vegetation and soil) changes with the density. At large pixel sizes, it is frequently aimed to map built up area. In urban areas, this is equal to the impervious surface. However, impervious surfaces can also occur outside of built up areas (e.g. transportation networks outside urban areas). For identifying built up area, an index is developed by Zha et al. (2003) for Landsat, analogue to the NDVI index for vegetation. The Normalised Difference Built up Index (NDBI) is defined as $(TM5 - TM4) / (TM5 + TM4)$, where TM4 and TM5 are the 4th and 5th Landsat TM bands, which are located in the near infrared (NIR, around 0.8 μm) and short wave infra red (SWIR I, around 1.6 μm). Especially in those spectral regions, the reflectance of built up area differs from that of vegetation and water.

Urban Structure

Urban structure provides insight in the configuration of the city and can be an indicator for social or environmental differences. With remote sensing urban structure can be mapped making use of the land cover, texture or spatial metrics. In Huang et al. (2007) spatial metrics are calculated on a land cover classification of Landsat data. They are calculated for 77 cities in various parts of the world. The aim of the study is to analyse urban form and analyse the differences among world regions and developed and developing countries. Several socio-economic development indicators were evaluated to gain more insight in the differences. The results of the study clearly show that urban agglomerations of the developing world are more compact than those in Europe or North America. In Herold et al. (2003) texture measures and landscape metrics are used to identify 9 different land use categories. The difference in texture and structure of the different land use types makes this possible. The landscape metrics are calculated on the results of a V-I-S classification of IKONOS data. In Stefanov and Netzband (2005) different landscape metrics were calculated from land cover maps to analyse the urban structure with respect to urban ecology.

Monitoring Urban Growth

Monitoring urban areas always contains a temporal aspect. For planners and scientists the growth of the city, the changes in building density and the decrease of vegetation density provide useful indicators for the dynamics of the urban area. In various studies changes are monitored with use of remote sensing. Madhavan et al. (2001) for example make a post classification comparison after mapping vegetation, imperviousness and soil with Landsat data to analyse the growth patterns of Bangkok. Durieux et al. (2008) uses an object based classification approach to identify buildings in SPOT data of different years. This is used to detect urban sprawl. In Zhang et al. (2002) a road density map (derived from remote sensing

data) is added to the spectral information of a Landsat image to reduce the spectral confusion between built-up and non-built up land cover categories. This additional information is used in a post-classification change detection to detect the change in built up area. In Zhang et al. (2002) also an overview of change detection approaches is provided. Among spectrally based methods for change detection, they differentiate between three main methods. In Table 3 an overview of those methods is provided.

Table 3: Three main categories of change detection methods after Zhang et al (2002)

Method	Description	References
Map algebra	Direct comparison of images of different dates using map algebra (e.g. differencing or rationing).	(Macleod and Congalton 1998; Sohl 1999)
Direct multi-date classification	A classification approach taking the images of both dates as one image data set, assigning classes such as 'change' and 'no-change'. Training of the classifier is based on both images.	(Li and Yeh 1998)
Post-classification comparison	The images of different dates are classified in compatible classification schemes and the classification results are compared. Relatively insensitive to changes in soil moisture and vegetation phenology.	(Mas 1999)

Risk Analysis and Vulnerability

With increasing size of cities, also the vulnerability of the cities for natural hazards increases. Various science disciplines are needed to provide complete information for risk analysis, vulnerability assessment or disaster management. Remote sensing has the possibility, in contrary to other sciences which for example use field surveys, to provide a complete view at least from the spatial perspective. Especially the physical parameters that contribute to knowledge on the vulnerability of an urban area can be provided with remote sensing (Taubenböck 2008). Examples of such parameters are building density, roof/house types, information on the accessibility and location (e.g. infrastructure, location of free spaces). Indirectly also land use can be assessed, which is important for assessing the risk: industrial areas are set out to other risks than residential areas. For assessing the risk of different hazards, of course different information is relevant. Taubenböck (2008) assessed the vulnerability of Istanbul, Turkey for an earthquake disaster. An object based classification approach of IKONOS data was used to identify land cover, building density and roof/house types. Bhaskaran et al. (2004) used HyMAP data to gather information to support post-disaster management after severe hail storms. A spectral angle mapper classification is carried out to identify areas that are vulnerable for future hail storms. The used classification scheme contains roofing materials with different vulnerability for hail storms. The derived information is incorporated in a geographical information system, to be combined with other information, e.g. on population distribution and cadastral information and provide that way emergency decision support information. With hyperspectral remote sensing, the mapping of hazardous materials such as asbestos becomes a possibility. After the attack on the World

Trade Centre in 2001, Clark et al. (2001) use AVIRIS data to identify hazardous clouds of asbestiform dust. The Tetracorder program (Clark et al. 2003) was used to produce material maps of the area. With use of field spectra, the variable amounts of chrysotile asbestos were determined and the materials could be mapped accordingly.

Urban Climate and Environment

The man made materials used in urban areas have significant influence on the urban (micro) climate (Kuttler 2004). The urban heat island phenomenon (UHI) is one of the direct effects of this climate modification (Oke 1987). Temperature is a suitable parameter to gain insight in the climatic situation. A relation between the land use or land cover and temperature is obvious and is a frequent research topic in urban remote sensing. Gluch et al. (2006) studied the relationship between surface temperature and surface cover with ASTER data. In this study, the land cover was modelled by the V-I-S concept at both urban and regional spatial scale. They found a decreasing surface temperature from dark impervious to soils to light impervious to vegetation. They conclude that the largest thermal emissions occur there where abundances of impervious surface were present. This indicates that impervious surface is also an important parameter for analysis of urban climate and the urban heat island. Also in Chen et al. (2006) the relationship between urban heat island and land cover was analysed. For the land cover classification a series of band indices is used on Landsat images. The used indices are Normalised Difference Vegetation Index (NDVI), Normalized Difference Water Index (NDWI), Normalized Difference Bareness Index (NDBaI) and Normalized Difference Build-up Index (NDBI). They found a positive correlation between NDBI and temperature and a negative correlation between temperature and NDVI, NDWI and NDBaI. Also Wilson et al. (2003) find a relation between NDVI and temperature. They demonstrate how this knowledge can be used in urban planning, by analysing different neighbourhoods and identifying developments with high and low impact on temperature.

Additionally, remote sensing can support the modelling of energy fluxes, e.g. by providing surface albedo (e.g. Frey et al. 2007; Govaerts et al. 2008). Hoyano et al. (1999) analyse the influences of urban form and materials on sensible heat flux. From the relevant parameter to model sensible heat flux, several could be mapped with remote sensing, such as urban spatial form (e.g. building geometry and density), surface albedo and materials.

Next to urban climate, also the environmental quality of urban areas gets more and more attention. Topics such as ecological quality and (environmental) sustainability are considered. For example material maps derived from hyperspectral data are used to support the mapping of urban biotope types (Heiden 2004). Bochow et al. (2007) uses a fuzzy logic approach to identify urban biotope types for each building block. In this study the urban biotope types are described by their materials, the building geometry, the imperviousness and vegetation. The study is a step in the direction of the automatic updating of urban biotope maps in Dresden, Germany.

5.3. Parameter Retrieval Strategies

The previous chapter has shown the broad application fields of remote sensing of man made surfaces. Many different sensors are used, depending on the application and availability.

With EnMAP a sensor type that not yet exists comes available: high spectral resolution and medium spatial resolution. Therefore in this chapter it is discussed what contributions EnMAP could make for each of the typical application fields. The different methods are evaluated with respect to their suitability for implementation in the planned EnMAP 'Toolbox'.

It should be kept in mind that urban areas are characterised by a high heterogeneity and relatively small objects. Many different materials with often distinct spectra occur next to each other. The small size of urban objects and according fast change of materials over short distances causes some problems. Many urban objects are smaller than one pixel of an EnMAP image ($< 30 \times 30 \text{ m}^2$). This results in many mixed pixels, making the identification of single objects or materials more difficult. A high spectral resolution allows the separation between those many materials. EnMAP is expected to be able to take care of the heterogeneity of urban and man made materials with its 200 spectral bands and its high signal to noise ratio.

5.3.1. Urban Land Cover/Land Use Mapping

In Table 2 frequently used methods for urban land cover classifications are listed. Those methods are all very flexible regarding the classification scheme. The more specialised classifications of materials and according to the V-I-S concept are addressed below. To take full advantage of the possibilities of EnMAP, research is needed to identify the most suitable classification scheme for urban areas, taking the sensor characteristics into account. For deriving an urban land cover map from EnMAP data a classification method should be selected that can make use of the high information content of hyperspectral data. Maximum likelihood classification and other traditional classifiers are not very suitable, since they cannot handle data with very high dimensionality. A data reduction applied on the hyperspectral data solves this problem, but can also cause a loss of information. A linear spectral mixing analysis would be the most suitable approach, because it provides a way to cope with the many mixed pixels that will occur in urban areas. However, it might be difficult to identify pure endmember spectra. A solution for this can be to use an external reference library with pure spectra of man made surfaces, measured with a field spectrometer or airborne hyperspectral sensor. The same problem of finding pure endmembers might also occur when using a spectral angle mapper approach or similar spectral comparison method. Support vector machines and neural networks can 'learn' also to recognise mixed classes, based on training areas, if the classes are selected suitably. That they retrieve very good classification results, also with hyperspectral data is shown by Waske and Benediktsson (2007) for SVM and Zhao et al. (2008) for neural networks. Zhao et al. (2008) claims that, though computationally more intensive, neural networks perform similar as SVM with small or moderate sizes of training data sets. A disadvantage is that both the training of neural networks and support vector machines require a lot of expert knowledge on how to set the parameters. A good user interface, e.g. as developed by Janz et al. (2007) may provide a solution for that.

Before applying any classification approach, it might be useful to de-shadow the image. The shadows cast by buildings will make it difficult to assign any class to the overshadowed area. Not many EnMAP pixels will be completely in shadow; however shadow will be a part of almost all of the mixed pixels. Experiments with de-shadowing algorithms such as described

in Richter and Müller (2005) are recommended to assess the potential enhancement of the imagery and the advantage of this for urban land cover mapping.

Material Classification

Materials are the most detailed level used for land cover studies in urban areas. Since the materials change at very small distances, not many pixels will contain only one material. Therefore a spectral linear unmixing approach is most suitable to identify materials. The spectral unmixing approach of Roessner et al (2001) is developed especially for urban areas. It uses a feature based classifier to identify the endmembers automatically from the image. Since it is trained with spectra of different German urban areas, the transferability to other western urban areas is promising. However, research is needed to prove if with 30 m spatial resolution still enough endmembers can be identified. Otherwise, a reference library might provide a solution.

Material identification methods not using spectral unmixing are based on the (manual) identification of endmembers and comparison of these with image spectra. Tools such as Spectral Angle Mapper (Kruse et al. 1993) or Spectral Information Divergence (Chang 2000) to make this comparison are essential when working with hyperspectral data.

V-I-S Classification

EnMAP is very suitable for a land cover classification according to the V-I-S concept. The scale level of the components fits to the 30 m spatial resolution of EnMAP. Up till now, land cover classifications according the V-I-S concept have mainly been carried out on multispectral data. The spectral information of this data turned out not sufficient to separate soil and impervious surface accurately, also not when the impervious surface class is replaced by a high and a low albedo class. Here the hyperspectral data will improve the results (Lu and Weng 2007). Most suitable is also here a linear spectral unmixing approach, with three or four endmembers. For example the approach of Weng and Lu (2007) could be implemented in the EnMAP Toolbox. A Minimum Noise Fraction (MNF) transformation is used to identify the endmembers. The four endmembers (soil, vegetation, high albedo and low albedo) are used in a spectral mixing analysis, deriving fraction images of each of the endmembers. In a next step a combined maximum likelihood and decision tree classification is performed to map land use and land cover, based on the fraction images. Sample plots from high spatial resolutions aerial photographs are used for training this hybrid classifier.

5.3.2. Urban Planning

For the application field of urban planning EnMAP can contribute to various parameters.

Imperviousness

For mapping the abundance of impervious surface with EnMAP data several approaches are suitable. Imperviousness is not represented by a dedicated spectral signature, but can be mapped by indirect approaches. One approach is the aggregation of impervious materials

into one class. For the identification of materials mapping approaches as discussed in section 0 can be applied. Another approach that is expected to retrieve good results with EnMAP data is that of Wu and Murray (2003). As explained in section 0 this approach is based on the V-I-S concept. After linear spectral unmixing of the members vegetation, high and low albedo and soil, the previous classes within the high and low albedo fractions are masked out (water, clouds, etc.). The sum of the high and low albedo fractions then provides the fraction impervious surface for each pixel.

As an alternative approach it would be interesting to study the possibilities of applying the Support Vector Machine approach presented by Esch et al. (2008) to simulated EnMAP data. The research should focus on the use of the full potential of the hyperspectral data in this method, which was developed for multispectral data. The approach needs detailed training data on impervious surface, e.g. from high resolution remote sensing data.

Buildings and Built-up Areas

To identify single buildings, the spatial resolution of EnMAP data will not be sufficient for most buildings. However, if a building map is available, the roofing materials might be identified with an unmixing approach. Especially here advantages are expected from data fusion and combination of data sets with different spatial resolutions. More research into this topic is necessary.

Built up areas might be best identified via impervious surfaces. The built up area index developed by Zha et al. (2003) for Landsat can be converted to the appropriate EnMAP bands. Since such an index is not taking advantage of the detailed spectral information available with EnMAP data, research into the possibilities of a hyperspectral built up area index might be interesting.

Urban structure

Urban structure mapping is often based on a land cover classification (e.g. Huang et al. 2007). However, texture measures can also indicate certain land cover /land use types (Herold et al. 2003). Using texture or spatial metrics as a tool for analysing EnMAP data would not make use of the full spectral information that the sensor provides. However, calculating spatial measures on land cover classification derived from EnMAP data might provide very good results. The higher the quality of the land cover classification, the more useful is the information derived by spatial measures. Especially when an urban area is frequently recorded by EnMAP, deriving a land cover map and sequentially spatial metrics can provide new interesting information for urban analysis. This could be an interesting application for future research.

5.3.3. Monitoring Urban Growth

EnMAP will have a revisiting time of less than a month in ideal cases. For urban analysis already a revisiting time of one year is very helpful. With currently available airborne hyperspectral sensors frequent overflights (e.g. once a year) over longer periods of time are expensive. EnMAP provides interesting possibilities for building time series and analysing urban growth and dynamics on a regular basis. For this, change detection methods are

necessary. Of the methods presented in Table 3, the post classification comparison approach is most suitable. The direct multi-date comparison will become very complex, when comparing images of more than two dates. Map algebra approaches compare the image spectra directly. Atmospheric correction is obligatory for this. Still, the comparison will only tell where the changes have occurred and not what the old and new land cover is. For the EnMAP toolbox, a post classification comparison tool is highly recommended.

5.3.4. Risk Analysis

For risk analysis EnMAP can contribute to land cover mapping (for methods see section 0 and 5.3.1) and to the estimation of building density, e.g. by applying texture measures on a land cover classification or the results of a built up area index (see section 0). For the identification of roof or house types, the spatial resolution of EnMAP will not be sufficient. However, EnMAP can contribute to the identification of abundance of hazardous materials, such as the identification of abundances of asbestos. More research is needed to make sure that quantitative spectral analysis, as is common for mineral and material mapping, works as well at medium spatial resolution.

5.3.5. Urban Climate and Environment

Until now most applications of remote sensing for urban climate analysis researched in the relation between temperature and land cover. Several relationships e.g. between building density and temperature or vegetation cover and temperature have been established. EnMAP data can be used to identify land cover and support urban climate analysis indirectly by the relation between land cover and temperature.

EnMAP data could also contribute to the modelling of urban climate. Short wave albedo can be derived by the EnMAP sensor. However, this will not make use of the hyperspectral potential, since in climatology mainly a broad band albedo is used (Frey et al. 2007). The identification of materials as input for climate models, of which the different characteristics also influence urban climate, can be a new field of application. So far, remote sensing is not often used for deriving material maps or material characteristics as input for climate models. Hyperspectral remote sensing is capable of identifying material abundances. Research into the use of material abundances and material characteristics derived from EnMAP data as input for climate models is recommended.

5.4. Priorities and Recommendations for Implementation

In the previous chapters an overview is given of the most important application fields of remote sensing of man made surfaces and how EnMAP can contribute to those fields. A summary of parameters relevant for analysis of man made materials to which EnMAP can contribute is presented in Table 3.

One of the most important parameters is urban land cover. This parameter is important in all application fields of urban remote sensing. There exist various classification schemes at different spatial scales. Research is needed to determine the most suitable classification scheme for EnMAP data, of course in respect to the application field. To identify land cover

classes smaller than the pixel size, which will be frequently the case in urban areas, a spectral unmixing approach is recommended. With many mixed pixels it might be difficult to find enough pure pixels to train a classifier, especially for the identification of materials. Therefore the implementation of a reference library of man made surface spectra in the toolbox is recommended. For mapping imperviousness, an important parameter for urban planning, it can be made use of the V-I-S concept. So far, this concept has been mainly applied to multispectral data, but significant improvements are expected from the use of hyperspectral data. For applications in urban climate analysis and risk analysis EnMAP can contribute with the identification material abundances, e.g. of hazardous materials. Large potential provides EnMAP for the monitoring of urban dynamics in time. The implementation of a change detection tool into the toolbox is therefore highly recommended.

With EnMAP a unique tool for the analysis of man made surfaces becomes available. The medium spatial resolution is suitable for mapping complete cities at once. The high spectral resolution makes it possible to identify the large variety of materials, which have distinct but small spectral characteristics. Last but not least provides the frequent revisiting time new and very promising possibilities for monitoring the dynamics of urban areas with hyperspectral data.

Table 4: Overview of recommended tools for the EnMAP Toolbox for analysis of man made surfaces

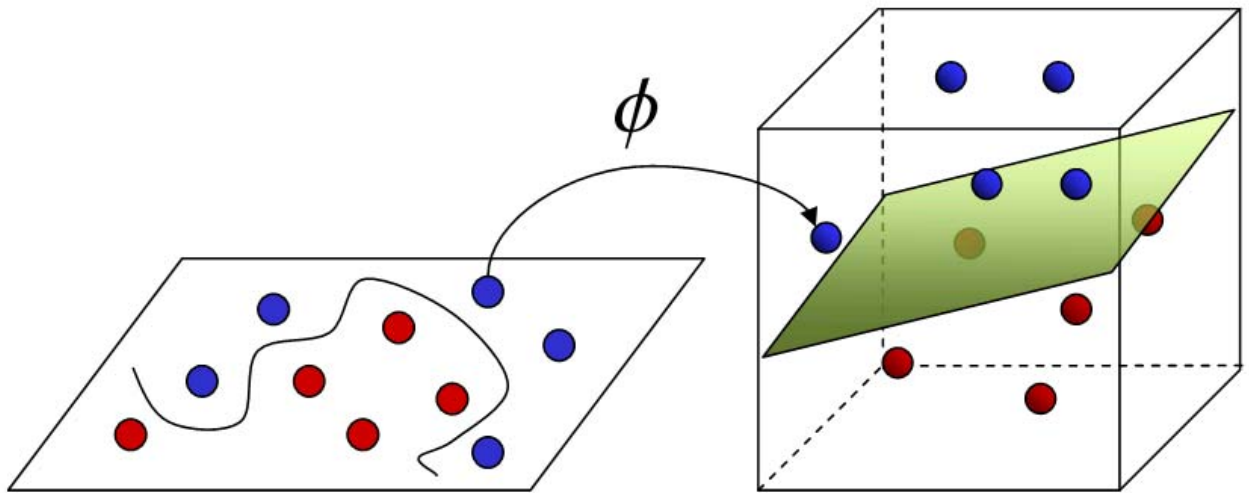
Parameter	Method/tool	Description	Research recommended	Reference
Urban land cover	Linear spectral unmixing	Classification approach takes mixed pixels into account and provides class cover fractions per pixel	Development of a suitable classification scheme according to spatial and spectral scale Research into the retrieval of endmembers from the image / need for external reference endmembers	(Lu and Weng 2006; Pu et al. 2008; Small 2003)
Urban land cover	Support vector machine	Advanced supervised classifier, possibility of taking additional data into account	Development of a suitable classification scheme according to spatial and spectral scale Research into the combination with high spatial resolution data	(Janz et al. 2007; van der Linden et al. 2007)
Material mapping	Linear spectral unmixing	Calculates material cover fractions based on endmembers automatically derived from the image by a feature based classification	Implementation and evaluation of the method to 30x30 m ² spatial resolution	(Roessner et al. 2001)

Parameter	Method/tool	Description	Research recommended	Reference
Material mapping	Linear spectral unmixing	Calculates material cover fractions based on endmembers automatically derived from the image by a feature based classification	Implementation and evaluation of the method to 30x30 m ² spatial resolution	(Roessner et al. 2001)
Material mapping	Spectral comparison tools	SAM, SID, etc.	Research into the retrieval of endmembers from the image / need for external reference endmembers	(Chang 2000; Kruse et al. 1993)
Man made surface endmembers	Field measurements or airborne hyperspectral remote sensing	Library of pure man made surface reference spectra to support endmember identification in EnMAP data of urban areas with few pure pixels.	Development of an approach to enhance the reference endmembers for the EnMAP data with image endmembers	
V-I-S	Linear spectral unmixing	Mapping of cover fractions of vegetation, high albedo, low albedo and soil	Implementation and evaluation of the approach on hyperspectral data	(Weng and Lu 2007)
Imperviousness	Linear spectral unmixing according the V-I-S concept	Based on the cover fractions of high and low albedo the impervious surface fraction is calculated	Implementation and evaluation of the approach on hyperspectral data	(Wu and Murray 2003)
Built up area	NDBI	(SWIR-NIR)/ (SWIR+NIR)	Adaptation and improvement of the index to make use of narrow hyperspectral bands	(Zha et al. 2003)
Urban growth / urban dynamics	Change detection	Post-classification comparison		(Zhang et al. 2002)
Risk assessment	Land cover mapping	See above.	See above.	See above
Hazardous materials	Material mapping	Mapping the abundance of hazardous materials such as Asbestos, approach see material mapping	Evaluation of the quality of quantitative spectral analysis at 30 x30 m ² spatial resolution	(Clark et al. 2001)

Parameter	Method/tool	Description	Research recommended	Reference
Urban climate	Land cover mapping, material mapping	See above	See above	See above
Climate modelling input parameters	Material abundances	See material mapping methods above	Analysis of the use of material abundances in climate modeling and climate-relevant material characteristics in material spectra	
Data enhancement	De-shadowing	Improves spectra effected by shadows cast by buildings and clouds	Evaluation of the effect of de-shadowing of building cast shadows on 30x30m ² spatial resolution	(Richter and Müller 2005)

6. Review of Generic Algorithms with relevance for the EnMAP Toolbox

Sebastian van der Linden, Pedro J. Leitão, Andreas Rabe and Patrick Hostert



6.1. Introduction

6.1.1. Hyperspectral data processing and image analysis

The digital processing of hyperspectral remote sensing data is challenging in a variety of ways and for manifold reasons. (1) The physical data size of hyperspectral data, also known as imaging spectroscopy data, increases linearly with the number of spectral bands. Therefore the analysis of hyperspectral data often poses problems to processing intensive approaches. (2) By covering the full spectral range between approximately 0.4 and 2.5 μm in narrow bandwidths hyperspectral data is affected by atmospheric absorption to a greater extent than multispectral data from sensors that avoid related spectral regions and acquire data in wider bandwidths. Such influences, e.g. narrow selective absorption of atmospheric gases or absorption in wider spectral regions by atmospheric water vapour, on the one hand require more sophisticated pre-processing. With regard to image analysis, on the other, advanced processing methods/approaches are needed due to the low signal-to-noise ratio of affected regions and frequent artefacts of water vapour correction. Such approaches need to be capable of dealing with noisy data and of separating relevant and irrelevant information effectively. (3) The information surplus of the quasi continuous spectral information is often represented in small absorption features that are superposed by general trends of spectra in the visible (VIS) to near-infrared (NIR) regions, e.g. small iron-related absorption features in spectral regions of increasing reflectance. The use of such features during analysis requires ways to effectively extract spectral information. (4) The high dimensionality of the spectral feature space of imaging spectroscopy data causes problems for many statistical (image) analysis approaches. At first, the high collinearity of adjacent spectral bands might impact results during statistical regression approaches. Moreover, the size of training data sets required during supervised statistical image classification approaches is directly driven by the number of features. The often time consuming and expensive process of training data collection is therefore more problematic than in multispectral analyses.

For several years, the algorithmic development of hyperspectral data processing was characterized by attempts to adapt existing methods to the special data requirements. Statistical image classification and processing chains such as the one suggested by Kuo and Landgrebe (2002b) (Figure) illustrate well how additional steps were performed prior to a maximum likelihood classification in order to make this method suitable for high dimensional data.

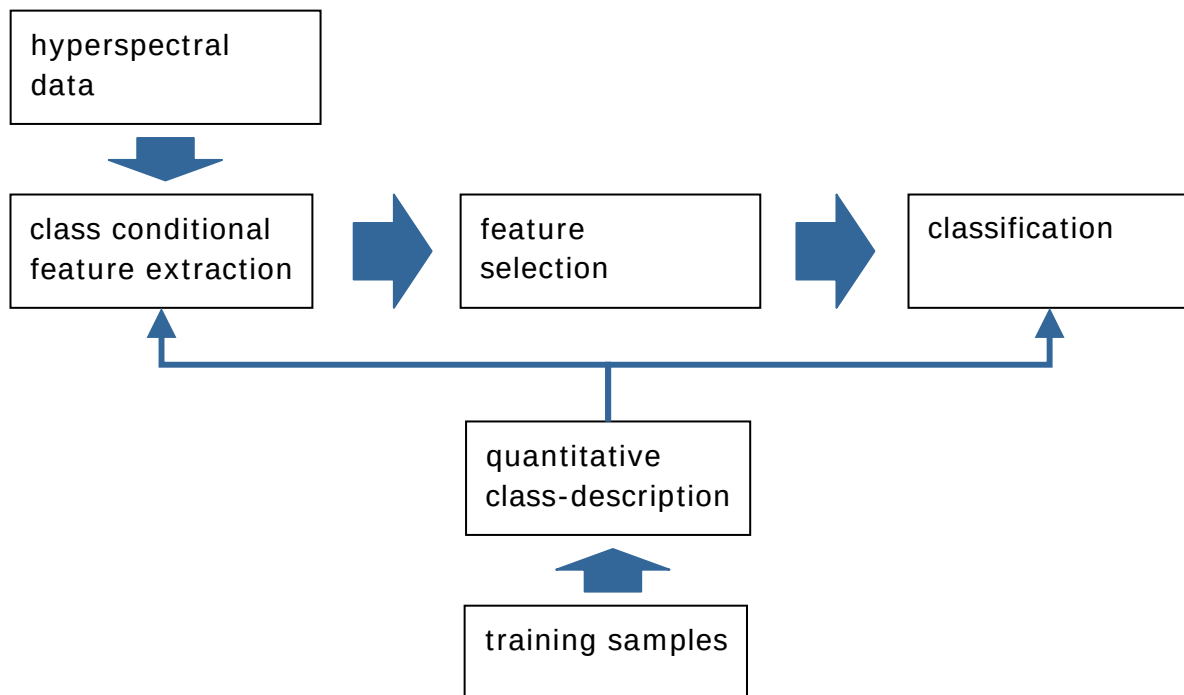


Figure 1: Schematic diagram for hyperspectral data analysis (Kuo and Landgrebe 2002b, modified)

Kuo and Landgrebe (2002b) suggest two additional processing steps, i.e. the class conditional feature extraction and a feature selection. In doing so, information that can be described by a normal or Gaussian distribution is extracted from the full range of spectral information and afterwards the most relevant features, i.e. features with highest discriminative power, are selected in order to limit the dimensionality of the feature space with regard to the size of available training data. When both steps are successfully completed, the calculation and inversion of the class-specific covariance matrix is possible, which is the central step in maximum likelihood classification. Such concepts appear very logical and have led to significant improvements in hyperspectral data processing (Dundar and Landgrebe 2004; Hsu 2007; Kuo and Landgrebe 2002b).

With regard to the complexity of the data processing workflow and this way to the processing power needed, such approaches are not favourable, however. Therefore a parallel development could be observed in hyperspectral image processing methodology, which is characterized by an increased use of machine learning algorithms that are not bound to certain assumptions on data distribution or less influenced by the dimensionality of the data. In the case of data classification - probably the most frequent analysis in remote sensing image processing – this parallel development started with the rise of artificial neural networks in the early 1990ies (Benediktsson et al. 1990). Looking at current literature, these approaches appear to experience a more and more frequent use and they seem to slowly replace approaches like the one displayed in Figure 1.

In this report the methodological development of generic algorithms for hyperspectral image data analysis is discussed based on a comprehensive review of publications in most relevant journals. The focus is on four main areas of data processing: feature extraction and selection (chapter 6.2.1), spectral mixture analysis (chapter 6.2.2), data classification (chapter 6.2.3), and data regression (chapter 6.2.4).

By focussing on these four areas, certain very relevant fields of hyperspectral image analysis are left out. Especially the wide field of radiative transfer modelling (RTM) is not addressed. However, RTM is best discussed in the context of certain applications, such as forestry or agriculture and it is therefore covered by other chapters of this joint report that show a clearer focus on applications. A similar case are spectral matching procedures; these are almost exclusively used in geological applications, where comprehensive spectral libraries exist, which are the basis for effective spectral matching.

6.1.2. Literature review

The following sections of this report are based on a comprehensive literature review. These scientific journals were considered:

Remote Sensing of Environment

International Journal of Remote Sensing

IEEE Transactions on Geoscience and Remote Sensing

IEEE Geoscience and Remote Sensing Letters

Photogrammetric Engineering and Remote Sensing

ISPRS Journal of Photogrammetry and Remote Sensing

International Journal of Applied Earth Observation and Geoinformation

Journal of Applied Remote Sensing

Within the databases of these publications for the period 1998 - 2009 (March) the following keywords were searched for: feature selection, feature extraction, band selection, spectral unmixing, MESMA, SMA, SVM, support vector, decision tree, random forests, neural network, ANN, classification, regression. The resulting list was filtered with a hyperspectral OR spectroscopy query in order to reduce the list of publications to hyperspectral applications. Based on the abstracts of the publications possible errors were eliminated, e.g. works on RTM that used neural networks for the inversion of the model. Moreover, papers with a clearly applied focus and missing information on the selected algorithmic approach were discarded.

6.2. Main Topics in Hyperspectral Data Processing

6.2.1. Feature extraction and selection

Overview

The topics of feature extraction (FE) and feature selection (FS) receive high recognition in remote sensing image processing, especially in the context of hyperspectral image processing, since FE and FS target at several of the challenges mentioned in Chapter 6.1.1. The following effects of the two methods can be summarized:

the number of features, i.e. original bands or derivatives thereof, is reduced

the collinearity or redundancy of features is (usually) minimized

This leads, in turn, to lower dimensionality and therefore less problems with the curse of dimensionality as well as a reduction in processing time.

Although the two terms are often mixed or used synonymously they shall be defined in two different ways for further discussion. *Feature Extraction* describes the derivation of new features which represent some information inherent to the original data. After performing FE a new data set exists which does (usually) not contain any of the original features/bands. *Feature Selection*, on the other hand, does not modify the original bands/features and simply selects a subset of original features. The two approaches may well be combined (e.g. Dundar and Landgrebe 2004; Kuo and Landgrebe 2002b), which is usually done in the order as they are explained here.

Both FE and FS are usually considered part of data preprocessing. In some cases, either one of the approaches is integrated in, for example, the classification approach and they can therefore not necessarily be seen as a separate preprocessing step (Archibald and Fann 2007; Bazi and Melgani 2006). Moreover, the selection of features may in a certain context be the objective of a scientific investigation and, again, FS would not appear as a preprocessing step but the actual core image analysis (Ferwerda et al. 2006).

Feature extraction is used (i) to represent the information inherent to a set of original features in a reduced set of newly generated features, e.g. by principal component analysis (PCA), wavelet transformation, or spectral indices, (ii) to extract non-linear dependencies between features, e.g. by kernel-PCA, or (iii) to approximate original information, e.g. when the spectral signal is approximated by a function. Moreover, operations such as spatial filters, can be used to generate texture measures, which constitute new features. Therefore the relatively new yet widely applied field of *image segmentation* can be regarded as a feature extraction procedure, when the segment measures are considered as properties of the original pixels.

Feature selection is used to reduce the set of (extracted) features to a smaller subset that (usually) contains a maximum of information with regard to a certain subsequent processing step such as image classification or regression analysis. FS methods can be divided into filter approaches, e.g. correlation analysis (De Backer et al. 2005; Goodenough et al. 2003; Gu et al. 2008a), and search approaches such as genetic search algorithm and/or forward/backward search (Archibald and Fann 2007; Kalacska et al. 2007; Keshava 2004; Martinez-Usó et al. 2007; Mutanga and Skidmore 2004; Pal 2006; Serpico and Bruzzone 2001; Serpico and Moser 2007). The latter may incorporate additional methods, e.g.

classifiers such as SVM or RF (Wang and Li 2008), in a wrapper approach (Kohavi and John 1998).

Literature on FE and FS with hyperspectral data is plentiful. For this review more than 50 publications were considered (see Appendix). Regarding the different hyperspectral sensors much of the work is performed using HyMap data (Camps-Valls et al. 2004; Deronde et al. 2008; Mutanga and Skidmore 2004) but various applications on AVIRIS, AISA Eagle, MERIS and Hyperion data exist as well (Archibald and Fann 2007; Deronde et al. 2008; Goodenough et al. 2003; Ham et al. 2005; Hsu 2007; Jia and Richards 1999). With regard to regional distribution, North America and Europe, but also Africa and Australia are represented in the literature. In general FE and FS is used for studies in most terrestrial biomes.

Feature extraction by data transformation

There have been approaches to further improve the “classical” PCA, e.g. by spectrally segmenting the spectral range (Jia and Richards 1999; Miao et al. 2007), and by including a kernel in form of a moving window (Gu et al. 2008a) or genetic algorithms (Yao and Tian 2003). Moreover, more sophisticated approaches for class specific data transformations that evolved in the 1990's have been introduced (Lu et al. 2007). However, a methodological focus for FE that emerges in a variety of application fields can rather be observed for wavelet transformation (Blackburn 2007; Deronde et al. 2008; Hsu 2007; Kempeneers et al. 2005; Li 2004; Pu and Gong 2004; Rivard et al. 2008; Serpico and Moser 2007). Another promising approach appears to be the use of morphological profiles (Plaza et al. 2005), which is currently experiencing relatively intense research. Individual works are heading for additional directions. Here FE based on matching pursuit (Hsu 2007) or an approach to merge highly correlated adjacent bands and to project these onto their Fisher discriminant can exemplarily be mentioned (Kumar et al. 2001).

Summarizing, wavelet transform appears the most generally applied approach in this field of FE.

Feature selection with filter approaches

FS with filter approaches share the idea of merging or selecting features/bands based on their information quantity or the correlation between them (Jiang et al. 2004). Among the various measures to compare bands, Guo et al. (2006) recommend the bands mutual information, i.e. a measure of statistical dependence between two random variables. Martinez-Usó et al. (2007) recommend clustering-based band selection. A good overview of various statistical measures to be used in this context is given in Miao et al. (2007), who also compare those to the FE by transformation (compare chapter: Feature extraction by data transformation). In general, the use of FS by filter approaches appears useful for implementation, due to the high value of FS for hyperspectral data. However, no “best” strategy or generally accepted strategy appears to exist.

Feature selection with search approaches

When search approaches are used for feature selection, a dichotomy exists between forwards selection, i.e. sequentially increasing the number of features, and recursive feature

elimination, i.e. sequentially eliminating features from the original set. Forward searches will start by identifying one most informative/discriminative feature and sequentially add more features, based on the same measure for information/discrimination (Deronde et al. 2008). Serpico and Moser (2007) modify three common strategies in this context, i.e. “Sequential forward selection”, “Steepest ascent” and “Fast constrained search” by first averaging groups of features, driven by the need to reduce extensive processing times of such statistical approaches. An effective example of recursive feature elimination, on the other hand, is given by Bazi, Y. and F. Melgani (2006), who include the feature selection directly into their classification approach. Other examples of such an embedding exist (Archibald and Fann 2007). Moreover various authors successfully integrate genetic search algorithms into FS (e.g. Vaiphasa et al. 2007; Yao and Tian 2003). Despite a clear direction or the existence of a “method of choice”, implementing a genetic search algorithm for matters of feature selection appears worthwhile.

Algorithm specific feature selection approaches

Another variant of Feature Selection, similar to those that embed the feature selection into the subsequent analysis, e.g. classification, are approaches that use algorithms like classifiers or regression analysis to identify most relevant bands. The Wrapper strategy as introduced by Kohavi and John (1998) for example is based on the idea to combine forward selection/recursive elimination with arbitrary classifiers/regressors. First attempts in using support vector classification (compare chapter 6.2.3) and support vector regression (compare chapter 6.2.4) at Humboldt-Universität zu Berlin appear promising.

Moreover, decision tree (DT) strategies (compare chapter 6.2.3) have been used to identify highly informative/discriminative bands (Wang and Li 2008). Pal (2006) uses SVM, DT and a combination of SVM with genetic algorithms to select features with highest discrimination power and compares the three approaches in terms of final accuracy and computational cost. However, neither in that study nor by this literature review a single main strategy can be identifier.

6.2.2. Spectral mixture analysis

Overview

Spectral mixture analysis originates in the field of chemometrics and is based on the idea, that a mixed target, e.g. a variety of land cover types covered by an individual pixel, appears in an optical measurement as a combination of the pure spectra of represented components, the so-called endmembers (EM), weighted by their abundance. Especially with the advent of hyperspectral remote sensing, spectral mixture analysis (SMA) has become one of the very common approaches for remote sensing image analysis. Nowadays, it still experiences frequent application. Given the quantitative nature of the results from SMA and its ability to extract slight spectral differences inherent in the signal of hyperspectral data sets, related approaches are very well suited and effective for hyperspectral analysis (Asner and Heidebrecht 2002).

SMA is used in a variety of fields. Geology should probably be mentioned first, as mineral identification based on SMA and spectral libraries was shown to be very effective already in the 1980's (please refer to the Geology Chapter of this joint report for a more detailed description of applications). Nevertheless, spectral mixture analysis or similar approaches

are still frequently used whenever quantitative assessments are to be performed, e.g. (sparse) vegetation abundance, species composition, transitions of soil types or soil properties (Huete et al. 2003), post-fire assessment, or in singular cases cloud removal (Gomez-Chova et al. 2007) and snow fraction mapping (Vikhamar and Solberg 2003). Moreover, SMA is often used to generate LC maps that show discrete distributions derived from the continuous SMA outputs (Goodman and Ustin 2007), to map LC at sub-pixel scale (Boucher and Kyriakidis 2006) or enhance the spatial resolution of images (Gu et al. 2008b).

The high number of methodological publications in the field of spectral mixture analysis underpins the frequent use of the approach in hyperspectral image analysis. More than 60 publications were considered in this study, including a large fraction on the issue of EM selection/identification. From a regional perspective, most applications are performed in the western part of the US. This is in parts based on the data availability for this region (AVIRIS) but also by some strong remote sensing laboratories that played key roles in the development of SMA based analysis schemes, especially the ENVI Processing Scheme (compare Geology Chapter). European studies are mainly based on HyMap imagery. Moreover some studies using space borne data from MODIS, MERIS (Gomez-Chova et al. 2007) or Hyperion (Huete et al. 2003) exist. In general, applications based on SMA are performed in all application fields and exist for most terrestrial biomes including benthic (Goodman and Ustin 2007) or urban areas (Franke et al. 2009).

Current literature rather shows the importance of EM related issues than further algorithmic development. Despite few non-linear approaches or extensions like derivative based unmixing (Zhang et al. 2004, 2005) or multitemporal SMA (Okin 2007), the linear mixing model prevails, probably because the underlying assumptions of linear mixing is in accordance with the desired applications outcomes. Attempts to introduce new approaches that overcome deficiencies of SMA, e.g. Mixture Tuned Matched Filtering to “unmix” single EM (Robichaud et al. 2007) or an unmixing approach that neglects the pure pixel assumption (Miao and Qi 2007) never reached high frequent usage. However, the general mixing model requires ideal EM sets for each pixel. Thus two main directions can be identified in current literature, (i) strategies for EM selection/ identification and (ii) the design of multiple models that adapt to spatial variations of the EM composition.

Approaches for endmember identification

Over the past years, several algorithms have been developed for autonomous and supervised EM extraction from hyperspectral data. Due to a lack of commonly accepted data and quantitative approaches to substantiate new algorithms, available methods have not been rigorously compared by using a unified scheme (Plaza et al. 2004). In general, methods that use both, spectral and spatial information are most effective (Plaza et al. 2004). Roessner et al. (2001), for example, introduce a method that reduces the number of possible EM combination for each pixel by introducing spectrally pure seedlings and a list of possible EM combinations into a neighborhood-oriented iterative unmixing procedure. Rand and Keenan (2001) partition the area using MRF to subset the EM selection. A similar approach, that uses a multiple EM spectral mixture analysis (compare chapter: Approaches for endmember identification) afterwards, has recently been developed (Schramm et al. 2008). In a spatial/spectral approach Plaza et al. (Plaza et al. 2002) use the concept of

mathematical morphology to identify locally pure spectra, in order to pay special attention to the high fraction of mixed pixels.

Approaches using multiple EM sets

The idea of multiple EM spectral mixture analysis addresses the problem of spatial heterogeneity in remote sensing data. Again, ideal EM subsets shall be selected for each pixels. This time, however, a finite number of complete EM combinations is considered and a best combination (not individual EMs as in chapter: 6.2.2 - Overview) is selected for each pixel based on a quality measure such as the root mean squared error or the maximum residual. The multiple EM spectral mixture analysis (MESMA) introduced by Roberts et al. (1998) is the most frequently applied strategy in this context. It was extended by additional strategies for EM subset selection criteria (Dennison and Roberts 2003) and has been applied in the context of post-fire assessment (Eckmann et al. 2008), tree species discrimination (Clark et al. 2005), vegetation abundance mapping (Okin et al. 2001). The MESMA concept was extended by Garcia-Haro et al. (2005) who added an additional stratification option to pre-select the EM combinations to be considered in certain areas. This approach called Variable Multiple Endmember Spectral Mixture Analysis (VMESMA) has not seen high frequent application in hyperspectral remote sensing, however.

An additional concept, similar to recursive feature elimination (compare chapter: Feature selection with search approaches) was introduced by Rogge et al. (2006). They start with a high number of possible EMs and iteratively reduce the EM set by the one EM that leads to the highest increase in model quality, e.g. based on RMSE. This Iterative SMA (ISMA) performs well in the original study but has so far not been evaluated by other groups.

6.2.3. Data classification

Overview

Data classification is the most relevant image analysis approach in remote sensing. Mapping terrestrial land cover (LC) or deriving information on the land use from remotely sensed signals has been performed for more than thirty years and it was one of the main drivers for methodological development of remote sensing specific digital image processing (Richards 2005). In chapter 6.1.1 of this review, a transition from traditional statistical approaches to approaches from the field of machine learning was outlined using the example of data classification. Despite a remaining high number of rather applied publications that still use statistical classifiers (Belluco et al. 2006; Cheng et al. 2007; Cochrane 2000; Deronde et al. 2008; Lu et al. 2007) the number of published works using approaches like support vector classification (SVC) or classification with self learning decision trees (DT) increases rapidly. With regard to hyperspectral data and its increased information content, the abilities of such advanced classifiers are used to further differentiate classification schemes, but also to classify thematically broad yet spectrally complex classes in a single step without further processing (van der Linden et al. 2007). This last issue shows the ability of advanced classifiers to handle multi-modal feature spaces. In this review, a strong focus is put on the two mentioned machine learning strategies, i.e. SVC and DT, as these appear to present state-of-the-art classification by time this report is written.

In general, data classification is used to map LC and this way derive discrete maps. The field of applications is therefore quasi infinite and nowadays extends as far as, for example,

mapping invasive species distributions (Lawrence et al. 2006) or mangrove zones (Held et al. 2003) and benthic systems (Hochberg and Atkinson 2003) based on hyperspectral data and DT or artificial neural networks, for example. Being the most frequent application in remote sensing and probably also in hyperspectral remote sensing, data classification is applied in almost any field of remote sensing, in all geographic regions and almost any biome. For this review 100 publications have been considered, including work from the Americas, Europe, Africa, Asia and Australia. In the same manner, image classification of every hyperspectral sensor exists, including CHRIS/Proba (Duca and Del Frate 2008).

Current research on data classification is as manifold as the number of methods and applications already existing. Richards (2005) gives an interesting overview on the state-of-the-art and the development he expects for the future decades. He mentions two issues. One is the use of fused data sets for LC mapping, that make use of the often complementary information contained in data from different sources. Applications of such fused data sets including hyperspectral data are becoming more frequent (e.g. Dalponte et al. 2008; Held et al. 2003; Koetz et al. 2008). The other direction he points out, is the use of SVC.

When data classification – here supervised classification - is discussed, one important issue has to be kept in mind: a classifier, including SVC and DT, is only as good (or bad) as its training data and results are evaluated only based on test data. Pal and Mather (2006) shed some light on this issue when discussing and comparing a variety of modern classifiers on hyperspectral data. Moreover, the mixed pixel issue, which constitutes one of the main arguments against image classification, has to be mentioned, whenever image classification is discussed. At this point, the work by Gamba et al. (2007) shall be mentioned, who separate mixed (boundary pixels) and in-object pixels and then apply separate classifiers with subsequent decision fusion.

In the following, state-of-the-art in data classification is discussed in five sections. At first, unsupervised classification is very briefly addressed, as it remains investigated yet never gained the importance of supervised classification. Afterwards SVC, DT and other supervised machine learning approaches are outlined, the first appearing as a quasi standard for comparison in recent methodological works. Finally, recent attempts to improve statistical classifiers by advanced processing chains are briefly addressed. It will not be attempted to describe all existing approaches but rather to show main directions and give an idea of the existing variety. Moreover, some works –not necessarily in hyperspectral remote sensing- combine methods from different areas to further improve results, e.g. by applying DT to intermediate results from SVC and this way further improve and stabilize classification results (Chen et al. 2008; Waske and van der Linden 2008).

Unsupervised approaches

Generally, classification methods are categorized, depending on the information available for the classifier design. The two main dichotomies are *unsupervised* and *supervised* approaches. During unsupervised classification or self-organizing learning systems (Chi and Ersoy 2005), the data are aggregated into natural clusters or classes that have similar properties, without having any additional knowledge, for instance from ground truth data. Widely used clustering methods are for example the ISODATA and the k-means algorithms

(Duda et al. 2001; Richards and Jia 2006). A general problem of unsupervised algorithms is that data may comprise clusters of different shapes and sizes. In this context, the definition of clusters and the selection of an adequate similarity measure are difficult (Jain et al. 2000). Another drawback for these algorithms is that the number of classes is usually unknown, because the clustering process considers feature classes instead of final information classes, i.e., land cover types.

The number of hyperspectral applications using such unsupervised approaches is relatively small. At this point the approach by Shah et al. (2004; 2007), who use an independent component analysis combined with a mixture model (ICAMM) to avoid the Gaussian distribution assumption, shall be mentioned, as it underlines the trend towards distribution free classification approaches. In a similar manner Filippi et al. (2006) use unsupervised artificial neural networks for vegetation mapping and further extend this approach by including a continuum removal procedure (Filippi and Jensen 2007).

Support vector classification

SVM are well known in the field of machine learning and pattern recognition (Vapnik 1998). The approach is based on an optimal linear separating hyperplane, which is fitted to the training samples of two classes within a multi-dimensional feature space. The optimization problem that must be solved is based on structural risk minimization. It aims at maximizing the margins between the hyperplane and the closest training samples, the so-called support vectors. Hence, the classifier only requires samples close to the class boundary and works well with small training sets, even when high dimensional data sets are classified (Melgani and Bruzzone 2004; Pal and Mather 2006). Other valuable properties of SVM are their ability to handle noisy patterns and multimodal feature spaces.

In the context of hyperspectral remote sensing, SVC was shown to outperform artificial neural networks (ANN) (Camps-Valls et al. 2004) or, for example a combined PLS (compare chapter: Partial least squares regression (PLS)) and linear discriminant approach (Wilson et al. 2004), and it has been successfully used in multitemporal and multisource studies (Camps-Valls et al. 2008).

Current literature focuses on the simplification of the general SVM concept for classification. In this context, it was shown that the selected decomposition method to apply the originally binary SVM to multiclass problems has no effect on the quality of results (Melgani and Bruzzone 2004) and that SVM can well handle multimodal distributions in a single processing step (van der Linden and Hostert 2009; van der Linden et al. 2007). Moreover, increase in accuracy and reliability of results was investigated using, for example, composite kernels (Camps-Valls et al. 2006), semi-supervised learning (Chi and Bruzzone 2007), or the inclusion of genetic algorithms into the selection of feature subspaces and SVM parameters (Bazi and Melgani 2006)

Decision tree classifiers

Decision trees (DT) are a non-parametric classification method, which can handle diverse data sets, including categorical variables. An overview on the DT concept is given by Safavian and Landgrebe (1991). The basic idea of this technique differs from other concepts in pattern recognition: Whereas most classifiers use the entire feature space at once and make a single membership decision per class, a DT is based on a multistage or hierarchical concept that does not necessarily include the entire feature space. During the training phase

the DT successively partitions the training data into an increasing number of smaller, more homogenous groups. That is done by producing efficient test rules, estimated from the training data. Due to its nature, this process might lead to a splitting of thematic classes into more than one final node.

Pal and Mather (2003) show that univariate decision at individual nodes are as good as multivariate decisions, but simple decision trees perform worse than ANN or maximum likelihood classifiers. Therefore more complex DT concepts were introduced, usually comprising ensembles of DT classifiers, that are trained in different ways and whose individual outputs are then combined into one final decision. This concept is applied, for example in Random Forests (Breiman 2001). In Random Forests (RF) two strategies for classifier ensembles, i.e. the bagging of samples and the random feature selection, are combined. Each tree within the ensemble is trained on a subset of the original training samples (bagging); in addition the split rule at each tree node is determined, using only a randomly selected feature subset of the input data (random feature selection). In doing so, a diversity of trees with different split rules is generated (Ham et al. 2005). This concept leads to results better than simple DT (Lawrence et al. 2006), is often comparable to boosted DT (Chan and Paelinckx 2008; Kawaguchi and Nishii 2007) and performs similar to SVC in selected studies (Pal and Mather 2003)

Other machine learning approaches

A variety of kernel based methods has been tested in hyperspectral image classification (Camps-Valls and Bruzzone 2005; Dundar and Landgrebe 2004; Kwon and Nasrabadi 2005, 2006), all of which use implicit representations of the feature space that are non-linear in the original feature space (compare chapter: Support vector classification). Moreover the use of Markov-Random-Fields is propagated in several works, e.g. combined with Bayesian contextual information (Jackson and Landgrebe 2002a) or for non-parametric density estimation (Neher and Srivastava 2005).

The use of ANN has not further increased over the past decade according to this literature study. ANN were successfully tested against statistical methods, e.g. maximum likelihood classification (Eddy et al. 2008) or linear discriminant analysis (Gong et al. 1997). However, they have never outperformed SVC and have a higher risk of performing sub-optimal trainings.

Combined statistical classifiers

As outlined in the introduction to this review, statistical classifiers do not represent state-of-the-art. Nevertheless, they are sufficient in some applications and might be modified to catch up to machine learning approaches, which sometimes causes higher computational effort, though. Roessner et al. (2001) developed an approach based on a combination of spectral classification and pixel-oriented unmixing techniques to facilitate sensible endmember selection based on the reflective bands of the DAIS instrument. This approach was further extended by including shape information (Segl et al. 2003).

The majority of works in this field use FE and/or FS procedures prior to maximum likelihood classification (Jimenez and Landgrebe 1999; Jimenez et al. 1999; Kuo and Chang 2007; Kuo and Landgrebe 2002a, b; Rivard et al. 2008; Zhang et al. 2006). Moreover, the problems of statistical classifiers are tackled using sparse covariance matrices, which can be inverted with less training samples (Berge et al. 2007; Jia and Richards 2002; Mayer et al. 2007), or

using adaptive covariance estimators (Dundar and Landgrebe 2002; Jackson and Landgrebe 2002b).

6.2.4. Data regression

Overview

Data regression is commonly used in the field of hyperspectral image processing. Regression analyses are mostly performed in quantitative studies and applied to derive continuous outputs. By delivering quantitative results, regression approaches are capable of producing maps that represent transient environmental changes at a high level of detail. The representation of such subtle changes is a relevant surplus of hyperspectral data compared to data at multispectral resolution and regression analysis is therefore an essential tool in the context of hyperspectral data processing.

Due to their quantitative nature, applications that use regression analysis for information retrieval cover a wide range of scientific fields, such as plant physiology (Coops et al. 2003), forestry (Pu and Gong 2004), agriculture (Hansen and Schjoerring 2003), species composition (Schmidtlein and Sassini 2004), pest management (Pontius et al. 2008), soil properties (Farifteh et al. 2007), or hydrology (Doxaran et al. 2005). In most cases, regression approaches are used to relate spectral surface properties to bio-physical (Ferwerda et al. 2005) or bio-geochemical properties (Galvao et al. 2008). Such approaches often include the identification or prioritization of relevant bands and therefore implicitly perform a spectral feature selection (Cho and Skidmore 2009). Moreover, when used to derive probabilities of certain phenomena, data regression may be part of data pre-processing, e.g. for noise or atmospheric correction (Roger and Arnold 1996; Sanders et al. 2001).

Literature on regression analyses with hyperspectral data is plentiful. For the scope of this literature review approximately 60 publications were considered relevant (see Appendix). From a sensor perspective, most publications are based on data from AVIRIS, particularly studies from the 1990s and early 2000s (Gaddis et al. 1996; Riano et al. 2002), and in more recent publications on HyMap data (Cho and Skidmore 2009; Schlerf et al. 2005). Few studies, however, make use of spaceborne data such as those from the EO-1 Hyperion sensor (Coops et al. 2003; Pu and Gong 2004). With regard to regional distribution, North America and Europe are best represented in the literature. Regression approaches on hyperspectral data have been, however, performed in most terrestrial biomes, including grasslands, savannas, wetlands, agricultural land, as well as various forest biomes, like broadleaf, Mediterranean, conifer or boreal.

Within the current research using regression analyses on this type of data, plant physiology studies (chlorophyll, water content, etc.) are the most prevalent. These methods are also commonly used for image pre-processing (Gaddis et al. 1996; Roger and Arnold 1996; Sanders et al. 2001), feature selection (Bajcsy and Groves 2004; Cheng et al. 2006; Cho and Skidmore 2009) and validation purposes (Monteiro et al. 2007; Mutanga and Skidmore 2004).

Many studies apply regression analyses for finding linear relations between known spectral indices or to identify suitable spectral indices, capable of describing specific (measured) target properties (Ferwerda et al. 2005; Noomen et al. 2008; Zhao et al. 2007). Other studies use continuum removal approaches for identifying absorption bands (through regression analyses) and thus the respective target components (Huang et al. 2004). Although most of these studies applied different forms of linear regression approaches, sometimes with a priori feature transformation (logarithmic, quadratic, etc.), some recent studies demonstrated the usefulness of non-linear approaches for resolving various problems, such as image pre-processing (Sanders et al. 2001) or biophysical estimation (Arenas-Garcia and Camps-Valls 2008).

From the studies reviewed, three main regression approaches are worth of notice, either by their frequent usage and ease of interpretation, such as (univariate and multivariate) ordinary least squares (OLS) analysis, or by their great potential to deal with such highly collinear datasets, such as ordination (principal component regression- PCR) or latent variable (partial least squares - PLS) methods.

Univariate and multivariate ordinary least squares regression - OLS

Most commonly, univariate regression methods have been used to quantify linear relations between specific band wavelengths or spectral indices and biophysical parameters. Such is the case of Ferwerda et al. (2005), where the authors identified species-specific spectral indices (band combinations) capable of describing plant nitrogen content. Similarly, Black and Guo (2008) used a previously-known spectral index (PRI - Photochemical Reflectance Index) to quantify and predict field-measured plant CO₂ exchange rate. Alternatively, multivariate methods can also be used, as in the study by Mutanga et al. (2004) where the authors make use of stepwise linear regression analysis for predicting plant foliar biochemical concentrations from continuum-removed absorption bands.

Multivariate regression analysis, however, is greatly affected by high-collinear data, which is an inherent characteristic of hyperspectral data. For this reason, and in order to validate the predictive capacity of such models bootstrap procedures need to be used (Ferwerda et al. 2006; Mutanga et al. 2004).

Implementations of ordinary least square regression analysis, including multivariate variable selection routines such as stepwise regression, exist on most commercially available statistical software packages, as well as on non-commercial (freely available) software environments like the R project for statistical computing (R Development Core Team 2009). IDL implementations also exist, like those of ITT's "IDL Advanced Math & Stats Module" and Creaso's "IDL Analyst".

Principal component regression (PCR)

One alternative regression approach which deals with the high in-between-band collinearity is the Principal Component Regression (PCR) analysis (Hotelling 1957; Massy 1965). This approach has been successfully used, e.g. by Gong et al. (2002) to estimate foliar nutrient contents of giant sequoia trees. Other authors have used this method for characterising

shallow lakes in terms of their chemical contents (Galvao et al. 2003) or for describing the mineralogical and chemical composition of tropical soils (Galvao et al. 2008).

This method consists in two analytical steps. First, a Principal Component Analysis is applied to the data, this way transforming the feature space into new linearly-independent factors, which are subsequently used in the regression analysis.

As with the previous, there are implementations of this method on both commercial and non-commercial statistical packages. IDL implementations of the Principal Component Analysis are available in both packages described above, which can be then combined with the regression analysis functions previously described.

Partial least squares regression (PLS)

However, probably the most interesting multivariate regression method for use with hyperspectral data is the Partial Least Squares (PLS) regression (Wold 1966). This method was applied, e.g. by Hansen and Schjoerring (2003) for measuring canopy biomass and nitrogen status in wheat crops. Also, Huang et al. (2004) applied it to the continuum-removed feature space to estimate tree foliage nitrogen concentrations from HYMAP data.

PLS regression is related with the PCR. However, in this approach, a first data transformation is applied to the full data space (features and response) with the constraint that the first resulting component, called latent variable, explain as much as possible of the covariance between the features and the response. After this first latent variable (or vector) is found it is subtracted from the data space and the process is re-iterated until reaching a null matrix and the full set of latent variables is determined. This way, the latent variables are orthogonal factors which have the best predictive power. This iterative process is then followed by a regression step where the decomposition of the transformed features is used to predict the response variable. A good description of this method is presented by Abdi (2007).

Due to the complexity of its functionality, implementations of this method are not as widespread as the previous. Nevertheless, some if not many (both commercial and non-commercial) software packages include PLS regression. Naganathan et al. (2008), however, present an IDL implementation of it in their study on the use of hyperspectral imagery for food quality assessment.

Other approaches

Other regression approaches have also been (less commonly) used on hyperspectral imagery. These include e.g. the logistic regression, used for image classification (Cheng et al. 2006). However, more advanced statistical approaches such as SVM or Artificial Neural Networks are expected to outperform logistic regression.

Penalized regressions methods, such as the Ridge regression, being suited to tackle high collinear datasets, can also be used with hyperspectral data, as in the study by Addink et al. (2007) who applied it to estimate vegetation biomass and LAI from HYMAP data. However these methods are neither easily implemented, nor are they as powerful as, e.g. the PLS regression.

Also, the non-linear extension of the PLS through the use of Kernel functions has been shown to be useful for feature extraction and dimensionality reduction in remote sensing applications, both for classification and regression problems (Arenas-Garcia and Camps-Valls 2008).

Finally, the **Support Vector Regression** approach, although it has not yet been applied to hyperspectral imagery, seems highly suited for this purpose as it makes use of the advanced machine learning capabilities of Support Vector Machines (as described above) applied to regression problems. Indeed, Xie et al. (Xie et al. 2008) use this method to estimate moisture transport in marine atmosphere from QuickScat and Multi-angle Imaging SpectroRadiometer (MISR) data. First attempts to use SVR on simulated EnMAP data at Humboldt-Universität zu Berlin appear very promising

6.3. Priorities and Recommendation for Implementation

In general, it is hard to recommend generic algorithms as remote sensing studies do always depend on the data, its quality, the region, the aim and type of application and so forth. Moreover, as described in previous chapters, many algorithms have been introduced, especially in publications with methodological focus, however, they are often not used by groups other than the one who developed it and can thus hardly be evaluated based on literature. Especially for Feature Selection algorithms and EM identification, this can be reported. On the other hand, some approaches can be reported that appear to be widely accepted, e.g. support vector approaches, decision tree approaches, wavelet transform and multiple EM unmixing approaches. Table 1 lists the most relevant approaches (according to this methodologically oriented literature review) sorted by the four main categories and explains the implementation status and importance of the method.

Table 1: Recommended approaches and implementations status/importance

Algorithm category	Approach	Implementation status/importance
Feature Selection/Extraction	Wavelet transform	Requires transfer to IDL; very useful
Feature Selection/Extraction	Wrapper approach (SVM/DT)	Exists in EnMAP Box by 12/2009
Feature Selection/Extraction	Genetic search algorithm	Requires transfer to IDL; very useful; tests required
Feature Selection/Extraction	Statistical search algorithm	not ideal for hyperspectral, yet probably desired
Spectral unmixing	V/ME/SMA	Basic method exists in ENVI, advanced elsewhere –
Spectral unmixing	Strategy for EM selection	Requires transfer to IDL; very useful; test required
Data classification	SVC	Exists in EnMAP Box
Data classification	DT (z.B. Random Forests)	Requires transfer to IDL; very useful
Regression	Univariate/multivariate OLS	Exists in EnMAP Box by 12/2009
Regression	PLS	Requires transfer to IDL; very useful
Regression	linear/non-linear SVR	Exists in EnMAP Box by 12/2009

7. References

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