Earth system science related imaging spectroscopy—An assessment

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The science of spectroscopy has existed for more than three centuries, and imaging spectroscopy for the Earth system for three decades. We first discuss the historical background of spectroscopy, followed by imaging spectroscopy, introducing a common definition for the latter. The relevance of imaging spectroscopy is then assessed using a comprehensive review of the cited literature. Instruments, technological advancements and (pre-)processing approaches are discussed to set the scene for application related advancements. We demonstrate these efforts using four examples that represent progress due to imaging spectroscopy, namely (i) bridging scaling gaps from molecules to ecosystems using coupled radiative transfer models (ii) assessing surface heterogeneity including clumping, (iii) physical based (inversion) modeling, and (iv) assessing interaction of light with the Earth surface. Recent advances of imaging spectroscopy contributions to the Earth system sciences are discussed. We conclude by summarizing the achievements of thirty years of imaging spectroscopy and strongly recommend this community to increase its efforts to convince relevant stakeholders of the urgency to acquire the highest quality imaging spectrometer data for Earth observation from operational satellites capable of collecting consistent data for climatically-relevant periods of time.

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1. Introduction/historical background

Three centuries ago Sir Isaac Newton published in his 'Treatise of Light' the concept of dispersion of light (Newton, 1704), indicating that white light can be dispersed in continuous 'colors' using prisms. The corpuscular theory proposed and developed by Newton was gradually succeeded over time by the wave theory, resulting in Maxwell's equations of electromagnetic waves (Maxwell, 1873). But it was only in the early 19th century that quantitative measurement of dispersed light was recognized and standardized by the discovery of dark lines in the solar spectrum by Joseph von Fraunhofer (1817) and their interpretation as absorption lines on the basis of experiments by Bunsen and Kirchhoff (1863). The term spectroscopy was first used in the late 19th century and provided the empirical foundations for atomic and molecular physics (Born & Wolf, 1999). Following this, astronomers began to use spectroscopy for determining radial velocities of stars, clusters, and galaxies and stellar compositions (Hearnshaw, 1986). Advances in technology combined with increased awareness of the potential of spectroscopy from the 1960s to the 1980s led to the development of first analytical methods (e.g. Arcybashev & Belov, 1958; Lyon, 1962); subsequently to the inclusion of 'additional' bands in multispectral imagers (e.g. the 2.09–2.35 \(\mu\)m band in Landsat for the detection of hydrothermal alteration minerals as proposed by A.F.H. Goetz); first imaging profilers (e.g. Chiu & Collins, 1978; Collins et al., 1982) and finally to initial research imaging spectrometers (e.g. Goetz et al., 1982; Vane et al., 1983). Significant progress was then achieved when, in particular, airborne imaging spectrometers became available on a wider basis (e.g. Cower et al., 1987; Kruse et al., 1990; Rowlands et al., 1994; Green et al., 1998), some of them helping to prepare for spaceborne imaging spectrometer activities (Goetz & Herring, 1989; Rast et al., 2001). However, true imaging spectrometers in space, satisfying a strict definition of a criterion of contiguity over an extended spectral range, either the visible near-infrared or through the shortwave infrared—as discussed later—are still very few. Recent developments indicate soon a larger availability of space based imaging spectrometers given the recommendation and/or approval of missions such as EnMap (Kaufmann et al., 2006) and the U.S. National Research Council’s decadal survey, which recommended implementing the HyspIRI mission (NRC, 2007).

Apart from technological advances, global modelers recognize that many of the key processes that control climate sensitivity or abrupt
climate changes (e.g., clouds, vegetation, oceanic convection) depend on very small spatial scales. They cannot be represented in full detail in the context of global models, and scientific understanding of them is still notably incomplete (Le Treut et al., 2007), and are asking for more holistic approaches at local scales. Airborne and spaceborne imaging spectrometers are currently targeted at providing solutions for the above issues. Nevertheless, imaging spectrometers may represent ‘the ultimate optical remote sensing technology’ that is very clearly not yet anywhere near complete’ (MacDonald et al., 2009-in this issue).

2. Definition

In the literature, the terms imaging spectroscopy, imaging spectrometry, hyperspectral imaging, and occasionally ultraspectral imaging are often used interchangeably. Even though semantic differences might exist, a common framework for such definitions is the simultaneous acquisition of spatially coregistered images, in many narrow, spectrally contiguous bands, measured in calibrated radiance units, from a remotely operated platform (Schaepman, 2007). Consequently, imaging spectrometer collected data facilitates quantitative and qualitative characterization of both the surface and the atmosphere, using geometrically coherent spectral measurements. This result can then be used for the mostly unambiguous direct and indirect identification of surface materials and atmospheric trace gases, the measurement of their relative concentrations, and subsequently the assignment of the proportional contribution of mixed pixel signals (e.g. spectral unmixing), the derivation of their spatial distribution (e.g. mapping), and finally their evolution over time (multi-temporal analysis).

3. Limitations and tradeoffs when using imaging spectrometer data

In many cases, the availability of a larger number of spectral bands has created important competitive advantages with regards to techniques based on multispectral imaging. In multispectral data, the detectable number of pure spectral signatures (endmembers) is often less than the effective number of endmembers present. In imaging spectrometer data, the effective number of spectral signatures generally exceeds the number of endmembers present in a pixel. This results in a tradeoff between these technology, a fact that introduces important limitations in the inversion process required to estimate the fractional abundances of spectral endmembers (Adams et al., 1995). In addition, the fine spectral resolution available in imaging spectrometer data allows a more subtle characterization of the spatial heterogeneity using spectral mixture analysis techniques (Plaza et al., 2004). However, spectrometers still suffer from significant band-to-band correlation, resulting in dimensionality issues and consequently reducing the total amount of available bands—even down to the level of multispectral systems (Chang & Du, 1999; Chang, 1999; Guo et al., 2006). In addition signal-to-noise ratios are still low in certain systems and even fractions of minimal noise might introduce considerable errors (Nischan et al., 1999; Okin et al., 2001). Data volume is another tradeoff to be considered when designing imaging spectrometers, mainly due to limited downlink capacities from satellites to ground stations. A detailed discussion on advanced data reduction possibilities is presented in the pre-processing section of this paper. Tradeoff discussions of advanced multiband imagers versus contiguous imaging spectrometers will persist to exist and will mainly be dominated by SNR and spectral fidelity issues.

4. Relevance and impact derived from the scientific literature

Imaging spectroscopy has had exponential growth over the past two decades in terms of referenced publications and associated citations (cf., Fig. 1). There is a good indication of the increasing relevance of imaging spectroscopy to Earth observations and its related research. We performed searches in altavista.com, and citations in scopus.com using combinations of keywords (e.g., hyperspectral, imaging spectroscopy, and imaging spectrometry) to illustrate this exponential growth.

A thematic separation of the search terms used in the above overview will be increasingly difficult in the future, since methods based on imaging spectroscopy are not exclusively applied in Earth observation, but also in space research (Clark et al., 2005), exobiology (Arnold et al., 2002; Kiang et al., 2007a,b), neurosciences (Devonshire et al., 2004), chemometrics (Fernández Pierna et al., 2004), amongst others (Gessner et al., 2006; Miskelly & Wagner, 2005).

A recent analysis using Scopus (Scopus, 2007) for remote sensing and imaging spectroscopy related articles (n = 74801, using search terms ‘imaging spectroscopy’, ‘imaging spectrometry’, ‘hyperspectral’, or ‘remote sensing’) resulted in an h-index (Hirsch, 2005) for remote sensing of h = 159 (indicating that 159 scientific contributions in remote sensing were cited at least 159 times), whereas imaging spectroscopy related articles contributed to h = 61 of these. Apart from textbooks and infrastructure articles being the most cited overall in remote sensing (e.g. Hapke, 1993; Holben et al., 1998; Jensen, 1996; Lillesand & Kiefer, 1979), imaging spectroscopy related topics are widely spread (n = 5810, using search terms ‘imaging spectroscopy’, ‘imaging spectrometry’, ‘hyperspectral’) and highly cited in a large variety of domains (e.g. Goetz et al., 1985; Green et al., 1998; Harsavala & Mustard 2002; Kruse 1993; Thenkabail et al., 2000).

5. Instruments

Earth observation based on imaging spectroscopy has been transformed in little more than two decades from a sparsely available
research tool into a commodity product available to a broad user community. In the latter half of the 20th century scientists developed spaceborne instruments that view the Earth in a few spectral bands, capturing a portion of the spectral information in reflected light. However, the few spectral bands of multispectral satellites fail to capture the complete diversity of the compositional information present in the solar reflected spectrum of the Earth. In the 1970s, realization of the limitations of the multispectral approach when faced with the diversity and complexity of spectral signatures found on the surface of the Earth, led to the concept of an imaging spectrometer. The use of an imaging spectrometer was also understood to be valid for scientific missions to other planets and objects in our solar system. Only in the late 1970s did the detector array, electronics, computer and optical technology reach significant maturity to allow creation of an imaging spectrometer. With the arrival of these technologies and scientific impetus, first generation instruments were proposed (e.g. Collins et al., 1982), with the Airborne Imaging Spectrometer (AIS) of the Jet Propulsion Laboratory (Vane et al., 1983) having most influence on the structural development of future imaging spectrometers. Even as a demonstration experiment, the success of AIS led to formulation and development of the proposal for the Airborne Visible/Infrared Imaging Spectrometer (AVIRIS), a system that measures the total upwelling spectral radiance in the spectral range from 380 to 2510 nm at ~10 nm sampling interval and an equivalent spectral response function (Green et al., 1998). The AVIRIS system has been upgraded and improved in a continuous effort since then to meet the requirements of investigators using hyperspectral data for science research and applications. Following the path initiated by AVIRIS, several new imaging spectrometers have been successfully employed in airborne (e.g. HyMap, AISA, Hydice, etc.) and spaceborne Earth observation based exploration missions (for a full listing of instruments see Schaepman, 2009). As a result, imaging spectrometer data today are widespread, but still not yet in common use. However, the lack of spatial and temporal continuity of airborne and spaceborne imaging spectrometer missions and data remains a recurring challenge to the user community. There is an emerging need to converge from exploratory mission concepts (e.g. former ESA's Earth Explorer Core Mission proposals such as SPECTRA; Rast et al., 2004), technology demonstrators (e.g. NASA's Hyperion on EO-1; Ungar et al., 2003), and operational precursor missions (e.g. ESA's CHRIS on PROBA; Cutter et al., 2004), towards systematic measurement and current operational missions (e.g. ESA's MERIS on ENVISAT; Bezy et al., 1999), NASA's MODIS (Salomonson et al., 1989) on Terra/Aqua). Despite the naming of MODIS (MODerate Resolution Imaging Spectroradiometer) and MERIS (Medium Resolution Imaging Spectrometer), these instruments follow the classical definition of “imaging spectrometers”, namely having more than 10 (narrow) spectral bands. Technically MERIS was built using a contiguity criterion, but end users do not receive contiguous spectral data products, whereas MODIS is built as an instrument with many (but not contiguous) spectral bands. Occasionally the term ‘hyperspectral’ has been suggested as an alternative for many band instruments, leaving “imaging spectrometer” for contiguous spectral bands instruments, but a literature survey on the use of these terms indicates a strong need for a proper terminology definition in this domain.

Several initiatives proposing space based Earth Observation instruments in these categories have been submitted for evaluation and approval (e.g. HERO (Hyperspectral Environment and Resource Observer; Hollinger et al., 2006), EnMAP (Environmental Mapping and Analysis Program; Kaufmann et al., 2006), Flora (Asner & Green, 2004), FLEX (Moreno et al., 2006), SpectraSat (Full Spectral Landsat proposal), MEOS (Trischchenko et al., 2007), amongst others). However for the time being, imaging airborne spectrometer initiatives (e.g. Asner et al., 2008a; Fournier et al., 2007; Kuester et al., 2007; Oppelt & Mauser, 2007; Richter et al., 2005; Schaepman et al., 2004) will continue to provide the majority of new instruments, before successor missions for Hyperion, CHRIS/PROBA and others are realized.

Finally, some promising new developments in instrument design for planetary exploration have potential application for Earth observations. A relevant ongoing effort in this context is the Moon Mineralogy Mapper (M3) (Green et al., 2008), selected as a NASA Discovery Mission of Opportunity in early 2005 and launched on October 21, 2008. M3 is the first imaging spectrometer designed to provide complete coverage of a planetary sized body in our solar system at high spatial resolution.

### 6. Technological advancement

Imaging spectrometer instrument technology will continue to benefit from various developments. Recently, true spectroscopy focal plane arrays have become available with improved quantum efficiency, increased readout ports, rectangular design and consistent readout in the spectral domain (Choriert et al., 2004; Chuh, 2004), also being expanded to the emissive part of the spectrum. To achieve high spectral–spatial uniformity and high precision measurements advanced optical designs require enabling components (curved, high-efficiency dispersive elements (Lobb, 1994; Mouroulis, 1998) and ultra-straight slits). Opto-mechanical designs must focus on spectral and radiometric stability (Xiong et al., 2005). With stability, spectral, radiometric and spatial calibration (Green, 1998; Green et al., 2003) can be readily established from the spectral features of the atmosphere as well as uniform/measured calibration targets on the Earth (Fox et al., 2003; Kneubuehler et al., 2004).

Complementing these instrument advances, new developments in high-performance computing will help overcome the limitations that current processing capabilities impose on certain imaging spectroscopy applications. In particular, the price paid for the wealth of spectral information available from imaging spectrometers is the enormous amounts of data that these instruments generate. Several applications exist, however, where having the desired information calculated in (near) real-time is highly desirable (Plaza et al., 2004). Such is the case of military applications, where a commonly pursued goal is detection of full or sub-pixel targets, often associated to hostile weaponry, camouflage, concealment, and decoys. Other relevant examples can be found in applications aimed at detecting and/or tracking natural disasters such as forest fires, oil spills, and other types of chemical contamination, where a timely response of algorithm analysis is highly desirable. In this regard, the emergence of programmable onboard hardware devices such as field programmable gate arrays (FPGAs) already allow real-time imaging spectroscopy data processing and lossless data compression in real-time (Mielikainen, 2006; Penna et al., 2006). On the other hand, the emergence of general purpose graphic processing units (GPUs), driven by the ever-growing demands of the video-game industry, have allowed these systems to evolve from expensive application-specific units into highly parallel and programmable commercial-off-the-shelf components which may eventually replace (more expensive) FPGAs as a tool of choice for onboard data processing and compression in many application domains with real-time requirements (Montrym & Moreton, 2005). Current GPUs can deliver a peak performance in the order of 360 Gigaflops, more than seven times the performance of the fastest ×86 dual-core processor (around 50 Gigaflops). The ever-growing computational demands of remote sensing applications will fully benefit from compact hardware components and take advantage of the small size and relatively low cost of these units as compared to FPGAs (Setoain et al., 2007). Despite the appealing perspectives introduced by specialized data processing components, current hardware architectures including FPGAs (which allow on-the-fly reconfiguration) and GPUs (fostering very high performance at low cost) still present limitations that must be carefully analyzed when

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1. [http://www.gpgpu.org](http://www.gpgpu.org)
considering their incorporation to remote sensing missions (El-Ghazawi et al., 2008; Woolston et al., 2008). In particular, the very fine granularity of FPGAs is still inefficient, with extreme situations in which only a very small portion of the chip is available for logic and effective algorithm implementations while the majority of resources need to be used for interconnects and configuration. This usually results in a relevant penalty in terms of speed and power. On the other hand, both FPGAs and GPUs are still difficult to radiation-harden (currently-available radiation-tolerant FPGA devices have two orders of magnitude fewer equivalent gates than commercial FPGAs).

Additional reduction in downlink volume may be realized by combining onboard processing capability with non-traditional data reduction techniques such as cloud screening, band aggregation (when appropriate for example in Case 1 water (ocean) applications), and employing smartly combined lossy and lossless compression (Abousleman et al., 1995; Aiazzi et al., 2001; Qian et al., 2006; Roger & Cavenor, 1996) over “stable” targets some of the time. With focus on these technological areas, spaceborne imaging spectrometers may be developed with user defined instrument performance (Schläpfer & Schaepman, 2002). Multiple-sensor approaches (Moreno et al., 2006), small satellites (Kramer & Cracknell, 2008), as well as imaging spectrometers sensitive in the multangular (Lee et al., 2007), thermal domains (Venius et al., 2006), and combinations thereof, will further significantly broaden the field of applications.

7. (Pre-)processing

A diverse array of techniques has been applied to extract information from hyperspectral data during the last decade (Chang, 2003). Pre-processing imaging spectrometer data is now adopting multi-instrumented approaches, including improved estimation of the composition of the atmosphere which allows retrieval of surface reflectance and ultimately the derivation of highly accurate Albedo products (e.g., blue/white-sky Albedo (BHR); black-sky Albedo (DHR)) (Govaerts et al., 2008; Schepman-Strub et al., 2006). On the other hand, processing techniques are inherently either full pixel techniques or mixed pixel techniques (Keshava & Mustard, 2002), where each pixel vector in a hyperspectral scene provides a “spectral signature” that characterizes the underlying materials at each site in a scene. The underlying assumption governing full pixel techniques is that each pixel vector measures the response of a single material (Landgrebe, 2003). By contrast, the underlying assumption governing mixed pixel techniques (also called “spectral unmixing” approaches) is that each pixel vector measures the response of multiple underlying materials at each site (Adams et al., 1986). Mixed pixels are a mixture of multiple substances, and may exist for one of two reasons. Firstly, if the spectral resolution of the sensor given by its point spread function is not high enough to separate different materials, these can jointly occupy a single pixel, and the resulting spectral measurement will be a composite of the individual spectra. Secondly, mixed pixels can also result when distinct materials are combined into a homogeneous, intimate mixture. This situation is independent of the spatial resolution of the sensor and its point spread function and therefore the issue of mixed pixels exists even at microscopic scales. An imaging spectrometer acquired scene (sometimes referred to as “data cube”) is therefore approximated using a combination of the two situations, where a few sites in a scene can be regarded as macroscopically pure materials, while most others are mixtures of materials.

An important aspect in the design of advanced imaging spectrometer image analysis techniques is how to efficiently integrate both the spatial and the spectral information present in the data. Most available techniques for imaging spectrometer data processing focus on analyzing the data without incorporating information on the spatially adjacent data, i.e., the data is treated not as an image but as an unordered listing of spectral measurements. In order to process the data without incorporating the spatial component, several single-pixel analytical techniques have been proposed. Principal component related techniques (Landgrebe, 2003) including mixture tuned matched filtering (MTMF), a method that estimates the relative degree of match of a given pixel to a reference spectrum and approximates the sub-pixel abundance, or partial least squares (PLS) regression models to characterize the variance in sample pixel spectra are widely used and have powerful applications in Earth System Science, including their use as pre-processing steps for further spatially-oriented processing. Additional efforts include modified Gaussian methods (Berge & Solberg, 2006) or wavelet-based methods (Kaewpijit et al., 2003). It is worth noting, however, that such spectral-based techniques would yield the same result for the data if the spatial positions were randomly permuted. In fact, one of the distinguishing properties of imaging spectrometer data is the multivariate information coupled with a two-dimensional (2-D) pictorial representation amenable to image interpretation. Subsequently, there is a need to incorporate the spatial component of the data in the development of techniques for imaging spectrometer data exploitation (Schaepman, 2007). Classification approaches are also changing from hard classifiers towards approaches of soft classifiers based on expert systems (Goodenough et al., 2000), Support Vector Machines (Camps-Valls & Bruzzone, 2005), Markov Random Fields (MRF) for sub-pixel mapping (Kasetkasem et al., 2005), contextual classifiers, and image change detection and fusion (Zurita-Milla et al., 2008). Further, morphological approaches for joint exploitation of the spatial and spectral information available in the input data have been recently explored (Clark et al., 2003; Dell’Acqua et al., 2004; Plaza et al., 2005; Soille, 2003).

While integrated spatial/spectral developments hold great promise for hyperspectral image analysis, they also introduce new processing challenges, especially from the viewpoint of their efficient implementation in (high-performance) computing platforms (Plaza & Chang, 2007). In particular, the price paid for the wealth of spatial and spectral information available from hyperspectral sensors is the enormous amounts of data that they generate. Several applications exist, however, where having the desired information in near real-time is critical. Such is the case of automatic target recognition for military and defense/security deployment (Chang, 2003). Other relevant examples include environmental monitoring and assessment (Phinn et al., 2008), urban planning and management studies (Roessner et al., 2001), risk/hazard prevention (Chabriott et al., 2002), assessment of health hazards (Kutser et al., 2006; Park et al., 2004; Thompson, 2002), detection of wildfire related events (Dennisson et al., 2006; Jia et al., 2006; Rahman and Gamon, 2004; Robichaud et al., 2007), biological threat detection (Russell et al., 2006), monitoring of oil spills and other types of chemical contamination (Flanders et al., 2006; Lopez-Pena & Duro, 2004; Salem et al., 2005). With the recent dramatic increase in the amount and complexity of imaging spectrometer data, parallel processing has become a tool of choice for many remote sensing missions, especially with the advent of low-cost systems such as commodity clusters. Further, the new processing power offered by grid computing environments can be employed to tackle extremely large remotely sensed data sets and to get reasonable response times in complex image analysis scenarios by taking advantage of local (user) computing resources (Brazile et al., 2008; Plaza et al., 2006). These advances will increase efficiency in processing data and meet timeliness needs (Wolfe et al., 2008).

Finally, there is a trend toward establishment of integrated systems solutions and supporting data assimilation (Dorigo et al., 2007; Fang et al., 2008) as well as data fusion based approaches (Gomez et al., 2001; Robinson et al., 2000; Zurita-Milla et al., 2008). These solutions are expected to provide scalable approaches, allowing the integration of multiple data sources. Data assimilation will further advance solid coupling of physical models, which link soil-vegetation-atmosphere-transfer (SVAT) models to state space estimation algorithms (Olioso
et al., 2005). Spectroscopy will be increasingly integrated into a multidisciplinary research environment, complemented by in situ sensing. Networks of in situ sensors exist already (e.g., FLUXNET), and with telecommunication technologies it is increasingly feasible for these networks to achieve (near) real-time integration of heterogeneous sensor webs into the information infrastructure (Andreadis & Lettenmaier, 2006; Schaepman, 2007).

8. Increased understanding of relevant processes through the use of spectroscopy

In this section, we discuss four main advances in remote sensing that have been achieved through the improved availability of air- and spaceborne imaging spectrometer data and related sciences. These are (i) bridging scaling gaps from molecules to ecosystems by using coupled radiative transfer models, (ii) assessing surface heterogeneity including clumping, (iii) physically-based (inversion) modeling, and (iv) interaction of light with the Earth's surface, respectively.

8.1. Bridging scaling gaps from molecules to ecosystems and biomes

Bridging temporal, spatial and spectral scaling gaps has always been a predominant topic in remote sensing (Chen et al., 1999; Marceau & Hay, 1999; Wessman, 1992), and their application to imaging spectroscopy has remained underexplored for a long time, but it now receives increasingly focused attention (Lewis & Disney, 2007; Roberts et al., 2004; Schaepman, 2007). While Malenovsky et al. (2007) discuss the topic in more detail, several approaches to bridge various scaling levels exist. Classical gaps can be identified in photon-vegetation interaction, when scaling from leaf to canopy level and coupled (or linked) radiative transfer models (RTM) are used (c.f., Jacquemoud et al., 2009—in this issue). Similarly, when scaling from canopy to ecosystem (or biome) level, coupled RTM including a full consideration of the atmosphere are needed (Baret et al., 2007). Other scaling approaches are based on using inverted geometrical optical models, where an estimate of the shadow and background fraction is needed for MODIS type spatial resolution (Zeng et al., 2008a,b). A more systematic coupling of these models will be needed to support scaling approaches ranging from leaves to ecosystems or even biome state assessment (Fig. 2) (e.g., Huang et al., 2007; Kobayashi & Iwabuchi, 2008; Malenovsky et al., 2008; Verhoef & Bach, 2007).

In the future particular attention will be paid to integrating plant physiological approaches from leaf to molecular level (Gierlinger & Schwanninger, 2007; Ustin et al., 2009—in this issue), and optimizing the coupling of canopy scale RTM with atmospheric RTM, supporting large region (semi-) operational retrieval of relevant surface parameters (Gobron et al., 2008; Pinty et al., 2007).

8.2. Assessing surface heterogeneity

The assessment of spatial heterogeneity—or canopy vertical and horizontal structure—has seen many approaches and today researchers are becoming increasingly interested in combined instrument approaches using LIDAR, multangular instruments and spectrometers to better address the structural complexity. Significant advances in assessing canopy heterogeneity using imaging spectrometers only have been achieved using the angular dimension of the data (Chopping et al., 2008) in addition to the spectral component. Even though model inversion and variable retrieval over closed canopies can be performed with reasonable complexity and good quality (Donoghue et al., 2007), sparse and clumped canopies are currently the greater challenge (Dauthoit et al., 2008) (c.f., Fig. 3). Much of the spectral mixture analysis literature using imaging spectroscopy addresses sparse vegetation conditions (Asner & Lobell, 2000; Asner et al., 2008b; Elmore et al., 2000; Garcia and Ustin, 2001; Mustard, 1993; Okiin et al., 2001; Roberts et al., 1997), scattering component separation (Roberts et al., 1993, 1998), and vegetation structure at the scale of functional type differences (Gammon et al., 1993; Pignatti et al., 2009).

Significant improvements have been made in identifying background (or understory) signals in sparse and clumped canopies (Bunting & Lucas, 2006) as well as refining the canopy composition at various levels of detail (Malenovsky et al., 2008). Additionally approaches using the advantages of full spectrum contiguous coverage have allowed the assessment of sparse and clumped forest canopies, given that some spectral separability is possible, either through dominant species occurrence (Schaepman et al., 2007) or unique biochemical species composition (Asner et al., 2008b).

In the future, we will increasingly see developing methods that either combine spectroscopic approaches with structural measurements

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Fig. 2. Coupled states, processes and scales ranging from cellular architecture to global biogeochemical cycles. The contribution of linked radiative transfer models in down-and upscaling ranges from leaves to biomes (modified following Miller et al., 2006).
Increasingly, systematic approaches using spectral databases (Bojinski et al., 2003) to serve as modeling baseline dominant species (Abbasi et al., 2008; Lucas et al., 2008) allow models to assess spatial estimates of carbon fluxes and pools (Quaife et al., 2006). Nonetheless, validation of models on forests of great structural complexity has not been demonstrated. Finally, due to the ill-posed nature of the inversion problem (Atzberger, 2004), a simplified approximation of the canopy representation may be required simply because larger numbers of variables will increase the uncertainty of the inversion.

Very few contributions discuss characteristics of old-growth forests (Song et al., 2002, 2007). In these studies, canopy structural variables and leaf optical properties were entered in a hybrid geometric-optical radiative transfer model (GORT) to mimic structural canopy changes characteristic of successional change. Fig. 5 also suggests a significant imbalance towards canopy biophysical properties compared to canopy (or even leaf) chemistry is observed. The retrieval of leaf chemistry is usually resolved by coupling a relatively simple leaf-level model (PROSPECT) with a canopy-level model (SAIL, DART, FLIGHT, GeoSAIL). The woody component is typically fixed in these retrieval studies, an assumption that does not necessarily match...(Asner et al., 2008c; Koetz et al., 2007a), advanced partitioning of various scattering properties (e.g., photosynthetic vs. non-photosynthetic vegetation; Verrelst et al., 2008, in revision), assessing canopy heterogeneity from spectrometer or using multiangular measurements (Gobron et al., 2002; Koetz et al., 2007b; Pinty et al., 2002) for pre-constraining RTM inversion procedures. Recent findings indicate the need for canopy representation at the shoot (needle) level, allowing proper upscaling approaches from leaves to canopies and biomes (Kokaly et al., 2009—in this issue; Zeng et al., 2008b).

8.3. Physical modeling

Quantitative, physical models have been widely used in remote sensing for all Earth system relevant spheres (e.g. soil (Pinty et al., 1989), vegetation (Koetz et al., 2004), snow (Painter et al., 2003), water (Hoge et al., 2003); atmosphere (Lyapustin, 2005), etc.). Imaging spectroscopy has significantly contributed to the accelerated use of physical models in remote sensing, fostered through the inherently high dimensionality of imaging spectrometer data (Boardman, 1989; Boardman, 1990; Hoffbeck & Landgrebe, 1996). Comprehensive comparisons of radiative transfer models used in remote sensing have been performed on a regular basis and document well the increased complexity incorporated in the modeling approaches (Pinty et al., 2001, 2004; Widlowski et al., 2007, 2008).

We further demonstrate the progress achieved in physical modeling on the retrieval of canopy characteristics using existing literature. The structure of the canopy determines the pattern of light attenuation and the distribution of photosynthesis, respiration, transpiration and nutrient cycling in the canopy (Baldocchi et al., 2004). Physically-based approaches to infer estimates of canopy characteristics from remote sensing data are increasingly used and have been shown to be useful, for example, in driving ecosystem models to assess spatial estimates of carbon fluxes and pools (Quaife et al., 2008), or biodiversity (Kooistra et al., 2008; Schaepman, 2007). Increasingly, systematic approaches using spectral fingerprinting of dominant species (Abbasi et al., 2008; Lucas et al., 2008) allow spectral databases (Bojinski et al., 2003) to serve as modeling baseline for inversion approaches. Fig. 4 shows the reflectance variability of 21,000 leaf measurements of dominant tree species performed in a heavily clouded area of the Elburz mountains region in Iran. Old-growth forests characterized by a structural heterogeneity and a large amount of woody compounds, may act as important carbon sinks (Knohl et al., 2003; Luyssaert et al., 2008). Despite the relevance of old-growth, however, a comprehensive review in Remote Sensing of Environment revealed that the majority of physically-based approaches have been applied on young to mature forests, rather than the more structurally complex canopies of old-growth forests. Fig. 5 displays studies of applications of RTM in the last decade. Radiative transfer models can be categorized as (i) 1D or turbid-medium models; or (ii) when the canopy space consists of crown architectural elements, as 3D model. In Fig. 5, the symbols indicate whether biophysical (open symbols) or biochemical (closed symbols) variables are quantified. At a glance, the suggestion by Huang et al. (2008) that relatively simple 1D models are still preferred is not confirmed by this figure. Some studies have evidently relied on the turbid-medium type of models such as the SAIL family (1D in space), yet the majority of the encountered studies effectively applied canopy models in 3D space. Mostly RTMs are usually linked with optical remote sensing data through numerical inversion methods with the purpose of inferring one or more model variable. For other applications RTMs are used to generate synthetic data e.g. for unmixing or classification purposes.

A model-driven motivation for selecting younger, structurally more homogenous stands may be the smaller degrees of uncertainty; hence these stands are better suited for model parameterization and validation. However, validation of models on forests of great structural complexity has not been demonstrated. Finally, due to the ill-posed nature of the inversion problem (Atzberger, 2004), a simplified approximation of the canopy representation may be required simply because larger numbers of variables will increase the uncertainty of the inversion.

Fig. 3. Assessing landscape heterogeneity of forest and agricultural canopies indicating the level of difficulty of the assessment (modified following Miller et al., 2006).
Fig. 4. Leaf spectral fingerprints of four dominant species in the Elburz mountains (Iran). Sunlit and shaded leaf measurements performed adaxial and abaxial along altitude gradients are plotted with their standard deviation.
8.4. From the interaction of light with the Earth surface to photon-matter interactions

Early classical remote sensing approaches were dominated by the qualitative interpretation of the interaction of light with matter (Gates & Tantraporn, 1952; Gates et al., 1965; Minnaert, 1940; Wakeling, 1980) and their interpretation of observations of the variety of colors and optical phenomena present in the atmosphere, water and the landscape. This interpretation of ‘color’ was gradually refined by using spectroscopic techniques, finally resulting in the assessment of photon-vegetation interactions (Myneni & Ross, 1991). This interaction approach has been continuously developed and modern imaging spectrometers currently provide observational validation of these early theories (Knyazikhin et al., 1992; Panferov et al., 2001; Shabanov et al., 2007; Widlowski et al., 2006). Also, single molecule spectroscopy is an emerging field (Michalet et al., 2007), with photon spectroscopy approaches being a realistic development in the near future (Bednarkiewicz & Whelan, 2007).

9. Contributions of imaging spectroscopy to the Earth system science

Imaging spectroscopy has not only enabled mapping parts of the Earth system with unprecedented accuracy (Adams et al., 1989; Ifarraguerri & Chang, 1999; Lee et al., 2004; Rast et al., 2004), but also significantly contributed to the mapping of its ecotones (Lucus & Carter, 2008) and other transitional zones (e.g. urban-green vegetation; Wania & Weber, 2007; Xiao et al., 2004).

In particular in unmanaged ecotones (e.g. ecosystem, communities, or habitat boundaries) like the tundra—boreal forest and forest—heathland transitions, are where pressure for change in terms of climate-related disturbance and human impacts are identified (Chapin et al., 2005). In managed (agricultural) ecosystems the improved precision is a key economical factor, contributing to better yield estimates (Zarco-Tejada et al., 2005) as well as use of high spectral and spatial resolution for species identification and mapping (Castro-Esau et al., 2006; Malenovsky et al., 2008).

In both managed and unmanaged ecosystems the spectroscopy focus is on detection and identification of plant succession, phenology, plant health, plant functional types (Schmidtlein & Sassn, 2004), and on monitoring invasive species (Asner et al., 2008c; Hestir et al., in press; Noudjina & Ustin, 2008; Underwood et al., 2003). Biochemical applications will concentrate on the (simultaneous) retrieval of moisture content (Cheng et al., 2006, 2008; Li et al., 2007), carbon (C) (Grace et al., 2007), nitrogen (N) (Martin et al., 2008; Smith et al., 2002), and potentially phosphorus (P) (Mutanga & Kumar, 2007), and connecting soil, leaf, and plant functioning with atmospheric fluxes using quantitative approaches. The pigment and photosynthetic system of vegetation is of increasing interest, which will finally allow coupling models from molecules to leaf, plant and canopy scales. The sound retrieval of combined atmospheric and vegetation properties will further allow refining 3D radiative transfer approaches in particular in partly cloudy atmospheres (Lyapustin & Wang, 2005).
Quantitative physically-based soil models remain to be developed taking into account the full spectral coverage (e.g. reflective and emissive) currently available, although many of the basic spectral interactions have long been a focus of interest (Stoner & Baumgardner, 1981).

Within the hydrosphere, imaging spectroscopy has supported the development of applications in aquatic environments (Schott, 2003), in particular within Case 1 (open ocean) (Morel & Belanger, 2006) and Case 2 (coastal) (Goodman & Ustin, 2007; Gitelson et al., 2008; Ruddick et al., 2001) waters, as well as inland water quality (Kallio et al., 2001) and bathymetry (Lesser & Mobley, 2007). Glacial surfaces, however, have been analyzed sparsely using imaging spectrometers so far, apart from instruments dedicated to outer space research (Doute et al., 2007).

Within the cryosphere, snow cover represents a critical component in Earth’s regional and global climate and hydrologic cycle. While the snow-albedo feedback is perhaps the most sensitive in controlling the Earth system response to changing climate, the albedo of snow across the globe is poorly understood and characterized (Dozier & Painter, 2004; Molotch et al., 2004). Recent advances in instrumentation, modeling, and scientific inquiry have substantially improved our understanding of the spatial and temporal forcing of and by snow cover. In particular, field and imaging spectroscopy have facilitated inference of the influences on broadband and hyperspectral directional reflectance of snow grain size (and in turn albedo), grain morphology, snow impurities, surface liquid water content, and biological content (Dozier et al., 2009-in this issue; Green et al., 2006; Matzl and Schneebeil, 2006; Nolin & Dozier, 2000; Painter et al., 2003, 2007a, b).

On the other hand, imaging spectroscopy of the lithosphere is very well established and in particular the interest in assessing the mineral composition of surfaces and materials advanced the development of spectroscopy most significantly. Mineral mapping can be identified as the most popular and successful application achieved using imaging spectroscopy, allowing various approaches to be implemented either focusing on the Earth (Clark et al., 1990; Cloutis, 1996; Kruse et al., 2003; Sabins, 1999) or other planets (Ribirino et al., 2005). Models of minerals were developed allowing key progress to be made in mixture analysis (Lucey, 1998) and topography (Feng et al., 2003). Beyond mineralogy, lithospheric approaches include mapping of volcanoes and their plume composition (Carn et al., 2005; Guinness et al., 2007; Spinetti et al., 2008) as well as indoor and outdoor dust analysis (Chudnovsky et al., 2007) and petrology (Edwards et al., 2007).

Within the pedosphere, assessing soil related variables receives significant attention. Topics such as mapping biological soil crusts (Ustin et al., 2009; Weber et al., 2008), mapping desert surface grain size (Okin & Painter, 2004), assessing soil carbon (Bartholomew et al., 2008; Okin et al., 2001; Stevens et al., 2006), separating soil and vegetation components (Bartholomew et al., 2007), and land degradation (Chabrillat, 2006) have become common. A detailed overview is discussed in Ben-Dor et al. (2008; this issue). However, physical based, quantitative models of soils beyond Hapke’s theory of the single scattering albedo remain sparse (e.g., Cerniewski & Karnieli, 2002; Liang & Townshend, 1996) and there is an urgent need for the development of such models, allowing soils to be treated in similar spectroscopy fashion as other Earth components.

The atmosphere has received significant attention with the use of advanced imaging spectrometers, either in measuring atmospheric composition (Bovensmann et al., 1999), or—related more to the observation of the Earth surface—the compensation of the atmospheric influence when deriving spectral surface properties from air- or spaceborne imaging spectrometers (Gao et al., 2009-in this issue; Liang & Fang, 2004). Atmospheric compensation or constituent retrieval will remain an ongoing challenge when separating surface and atmospheric scattering components (Gao et al., 2009-in this issue; Liu et al., 2006; Neville et al., 2008; Sanders et al., 2001; Qu et al., 2003).

Finally, within the Earth system sciences, integrated, multidisciplinary (or even transdisciplinary) approaches where imaging spectroscopy plays an important role will increase in frequency and impact. Environmental systems analysis with the support of imaging spectrometers can be found in various domains (Kokaly et al., 2007; Phan et al., in review), however true integrated approaches of Earth system science using imaging spectrometer data are still infrequent today.

10. Conclusions and outlook

Over nearly three decades, imaging spectroscopy has evolved from experimental approaches in their infancy to becoming a commodity product that is used in a multitude of Earth Science and Planetary Science applications.

Practically, to achieve new success requires improved data quality and wider availability of systematic and consistent remote sensing observations to the user community. Secondly, broader availability of high-performance distributed computing resources is also needed in order to run quantitative, physically-based models at various scales. Particular advances in the understanding of the interaction of light with the Earth surface and atmosphere have been achieved through coupled RTM bridging spatial, temporal and spectral scaling gaps from molecules to ecosystems and biomes. Spectrodirectional measurements incrementally improved the understanding and assessment of surface heterogeneity vertically and horizontally including clumping effects. The vast number of spectral bands in these instruments has allowed significantly improved physically-based (inversion) modeling. Ultimately our understanding of the interaction of light with the Earth surface has moved away from the classical color theory towards a more comprehensive understanding of photon-matter interaction. Our quantitative understanding of photon-matter interactions has been significantly enriched by the opportunity to look at simultaneous acquisition of many, contiguous spectral bands. Data fusion and assimilation methods will continue to increase the potential of these approaches, allowing the continuous assessment of the Earth system in the spectral, spatial and temporal domains. Summarizing all of the above, imaging spectroscopy currently enables spatially continuous mapping of physical, chemical, biological and artificial variables of the Earth’s surface and atmospheric composition with unprecedented accuracy.

In this paper, we have demonstrated the development and progress of significant new fields of remote sensing technology and applications and identified potential near-term advancements of imaging spectroscopy in the Earth sciences. However, the imaging spectroscopy community must increase its efforts to inform relevant stakeholders of the value of these data and the urgent need to acquire continuous high quality imaging spectrometer data of the Earth. The observed research trends indicate that this need is becoming more widely understood and seen as essential for the sustainable development of our resources and the protection of our environment. Various position papers underline the urgency of the above requirements, namely the requirement for consistent observations for long periods and more holistic instrumented approaches (Simon et al., 2006) that are capable of performing true multidisciplinary approaches to solving problems in the Earth sciences.

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