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A critique of field spectroscopy and the challenges and opportunities it presents for remote sensing for agriculture, ecosystems, and hydrology

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ABSTRACT

From the early scanning spectrometers, the utility field spectroscopy has been constrained: by detector sensitivity, leading to high integration times; portability; and the measurements having very limited support (possibly an Earth surface area in the order of 0.25m² to 2m²). However, over the last twenty years or so detector sensitivities and electronics have improved leading to practical Earth surface sampling time increasing their utility to support Earth observation science and as optical remote sensing teaching and training tools. Now the uncertainties associated with field spectral measurements are being more widely recognised and field sampling methods and instrument continue to be developed to enable these uncertainties to be quantified and minimised. There are a number of key challenges which still need to be more widely addressed if field spectroscopy is to provide evermore reliable and replicable measurements. An understanding of the systematic biases introduced by this sampling method has begun to be recognised. In addition, the mismatch in scale between near-ground spectroscopy measurement and observations from space-borne sensor has begun to be addressed with the development of unmanned aerial vehicles as platforms and lightweight and miniaturised state-of-the-art spectrometer systems. It is now possible to non-invasively sample terrestrial and hydrological ecosystems in a statistically robust manner and do so with supports similar in scale to those of air- and space-borne sensors. These developments will revolutionise the use of field spectroscopy to support empirical science and model development and the calibration and validation of space-based observations.

Keywords: Field spectroscopy, unmanned aerial vehicles, remote sensing, Earth observation scaling issue, spectrometers, DFOV and SFOV measurement modes

1. INTRODUCTION

In the 17th century Newton demonstrated that the colour of an object was an interaction of both light and object, although he appears to have been more interested in the nature of light than the colour of objects [1]. However, his work forms the foundation of optical physics and, consequently, the basis of the physical principles of spectroscopy. There is then evidence in the early modern French scientific literature (circa 1700) that relationships between the colour of leaves and their composition was being investigated [2, 3]. However, instruments capable of recording spectral data were not available at that time as neither photographic nor electronic recording media had been developed. Fast tract to the early 20th century and spectroscopic instruments were in evidence in scientific laboratories, although primarily in investigations in to human vision [4, 5]. The history of spectroscopy since then has been of increasing precision, accuracy and utility as there have been improvements in the technologies available to “disperse incident light energy into its constituent wavelengths and then detect and analyse this energy” [6]. The fundamental principle underlying spectroscopy, is that: a) when light interacts with any surface there is a photon energy level and flux density change; b) the light measured by the spectrometer will contain information on the light source, the atmosphere through which the light has passed, and the surface with which it has interacted. Therefore, light can be used as an 'information' carrier and from this information it may be possible to infer or estimate some properties of the media (atmosphere and surface) with which it has interacted if information of the source is known. So in spectroscopy it is the energy level, indicated by wavelength, and photon flux density per unit time (radiant flux), often in relation to some standard reference providing information of the light source, that is measured. Attempts are then made to relate the photon flux density per wavelength interval to physical properties of the media and to spectral measurements made by other investigators separated by space and time.

In the 1950's the potential of spectrally sampling the Earth's surface from airborne platforms was realised. Consequently, through the 1960s field spectrometers began to be developed albeit either scanning instruments, with limited resolution

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and sensitivity, or recording a limited number of bands and both with limited spectral range, to better understand the interaction of light with Earth surfaces and further understand the airborne images [6]. With the dawn of the space age, there was the realisation that the Earth's surface could be classified using spectral information and these space-based observations could provide unprecedented insights into ecosystem distributions, Earth system process, and surface physical and chemical properties [7]. This drove forward the development of field spectroscopy as: a) there was a need to better understand the optical properties, both spectral and directional, of Earth surfaces and the properties that could be inferred from spectral measurements and; b) there was a need to calibrate and/or validate (cal/val) space-based observations. These cal/val needs arise because spectral sensors on satellites record 'at-sensor' radiance and the light will have interacted with the Earth's atmosphere after leaving the surface, it will therefore carry information of these interactions as well as the surface information of interest to scientists. These interactions need to be accounted for. In addition, the calibration and stability tests performed before launch must still be verified after launch and, particularly, as the sensors age. Field spectroscopy and field spectrometers have therefore developed to increase our understanding of the interaction of light with Earth surfaces and as a method of calibrating or validating observations from air- or space-borne sensors [8].

With early scanning spectrometers, field work was constrained by detector sensitivity, computing power, power consumption, portability and many other factors. However, over the last twenty years or so instruments have become ever more sensitive, reliable and portable, leading to increasing use both to support science and as optical remote sensing teaching and training tools. Detector materials and technologies in particular are progressing. Photodetectors with sensitivities 1,000s greater than those currently used are now being reported [9], although it may take some time for these advances to be incorporated into field spectrometers. However, different instrument designs, field measurement methods and inherent uncertainties need to be considered when developing field sampling strategies to further improve the utility of field spectroscopy. The uncertainties associated with field spectral measurements are now more widely recognised [10]. However, it is worth emphasising that field spectroscopy is normally a passive remote sensing method relying on the highly dynamic and ever changing skylight, as can be seen from Figure 1a, as the source of illumination. As the energy level and flux density from the source changes so too will the reflected radiance being measured. This leads to a number of key challenges which need to be addressed if field spectroscopy is to provide reliable and replicable measurements. For example: minimising or avoiding a time lag between field reference measurement and target surface measurement; minimising the duration of the measurements (instrument integration time); relationship of the field reference standard used to those standards used by other investigators and their consistency (are they maintained, clean and calibrated to national standards?), all need to be considered. Much progress has been made and state-of-the-art field spectrometer systems and field methodologies are being developed to address these issues.

One major further constraint on the utility of field spectroscopy has been the size of the field measurement support and the significant mismatch in scale between this and the air- and space-borne observations – the so called 'Remote Sensing Scaling Issue' [11]. However, in the last two or three years even this issue has begun to be addressed with the development of small rotary-wing unmanned aerial vehicles (sUAVs) as platforms for lightweight and miniaturised spectrometers controlled by microcontrollers or miniature computers. It is now possible to non-invasively sample terrestrial and hydrological ecosystems in a statistically robust manner and do so with supports similar in scale to those of air- and space-borne sensors. These developments will revolutionise the use of field spectroscopy to support empirical science, as well as the development and validation of models. This is the key point that will be elaborated here.

2. FIELD SPECTROSCOPY MEASUREMENT MODES

Measurements of both down-welling irradiance (the reference measurement) and up-welling radiance (target surface measurement) can be carried out either in sequence (when a single spectrometer is used) (Figure 2), or simultaneously (when two separate spectrometers are used) (Figure 3). These are termed single field-of-view (SFOV) or dual field-of-view (DFOV) configurations, respectively. Both have advantages and disadvantages. As SFOV systems generally have a single spectrometer, they will normally be of a lower cost to set up than a DFOV system which requires two spectrometers. With a SFOV system there is also no need to inter-calibrate a spectrometer pair. However, long-term and unattended measurements with a SFOV systems face the challenge of automating a single spectrometer to measure both down-welling and up-welling radiation. This automation usually involves moving parts [12], which may become a problem for long-term field operation. It also entails a time delay between up-welling and down-welling measurements, which may introduce errors as can be inferred from Figure 1 and discussed previously. Similarly, DFOV systems have also associated advantages and disadvantages. Because photodetectors are temperature-sensitive [13], a system based on two spectrometers can be sensitive to temperature as each detector may be at a different temperature and have a different

radiometric response. One approach to alleviate this problem is to keep the two sensors at constant temperature by housing them in a temperature-controlled enclosure [14]. This may add significantly to the complexity of operation, not least as regular inter-calibration of the both sensors will be required, and to the cost. These limitations are partly overcome with a new single spectrometer DFOV system recently developed at the Field Spectroscopy Facility (Figure 10) and discussed further later in this article. However, the optical design of spectrometers and the method of light entering the spectrometer and being transferred to the detectors also needs to be considered.

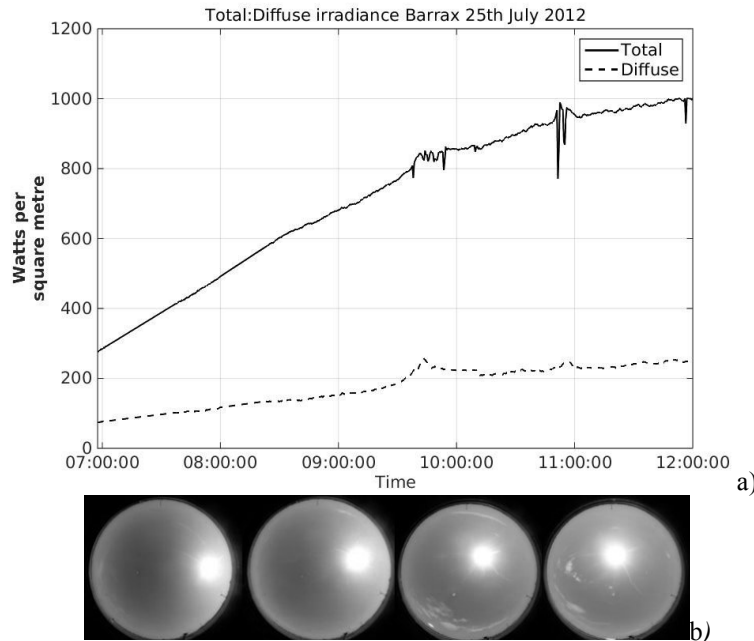


Figure 1a. Change in total and diffuse irradiance over a 5 hour period, b) selected concurrent sky hemispherical photos

3. INSTRUMENT-INTRODUCED SPECTRAL SYSTEMATIC BIAS

A number of publications are available which advise on procedures for radiometric calibration and the quantification of electronic system measurement uncertainties [15]. However, little work has been done to characterise the field-of-view (FOV) and responsivity of field spectroradiometers to radiant flux across this FOV. In the spatial sampling of Earth surfaces the ‘size, geometry and orientation in space’ of each area sampled is the support for subsequent analysis [16]. In Earth observation where images are acquired by remote sensing, and where complete coverage of an area is achieved, the support of each sample area is represented by pixels and the measurement of the support is effected by the sensor’s point-spread function (PSF) [17]. The PSF of an imaging system is reasonably well approximated by a two-dimensional Gaussian responsivity distribution [18] equally distributed radially over the support. The PSF delimits the area that is sampled and the weighting that the sensor assigns to the radiant flux from each reflecting element within the defined area. It has been demonstrated that the PSF has a significant influence on the information that can be derived from satellite images on a per pixel basis. However, although many sources discuss the characteristics of the PSF and instantaneous field-of-view (IFOV) of imaging systems little research has been published describing the corresponding phenomena for spectroradiometers. The general assumption has been that the FOV of a spectrometer, defined by the nominal solid angle specified by manufacturers for each fore optic, delimits the area of support. Therefore, elements within this area, contributing to the measured radiant flux, can be identified and quantified. That the area delimited by the FOV is considered to define the support for subsequent analysis is demonstrated when elements within the instruments’ FOV; the ground FOV; the diameter of the FOV; the footprint; and the area observed by the sensor, are referred to in the literature.

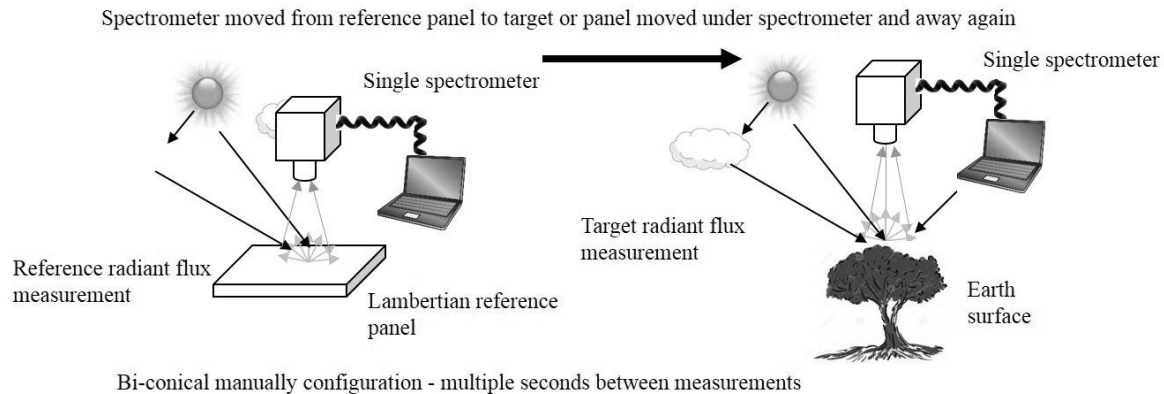


Figure 2. Single spectrometer single field-of-view mode

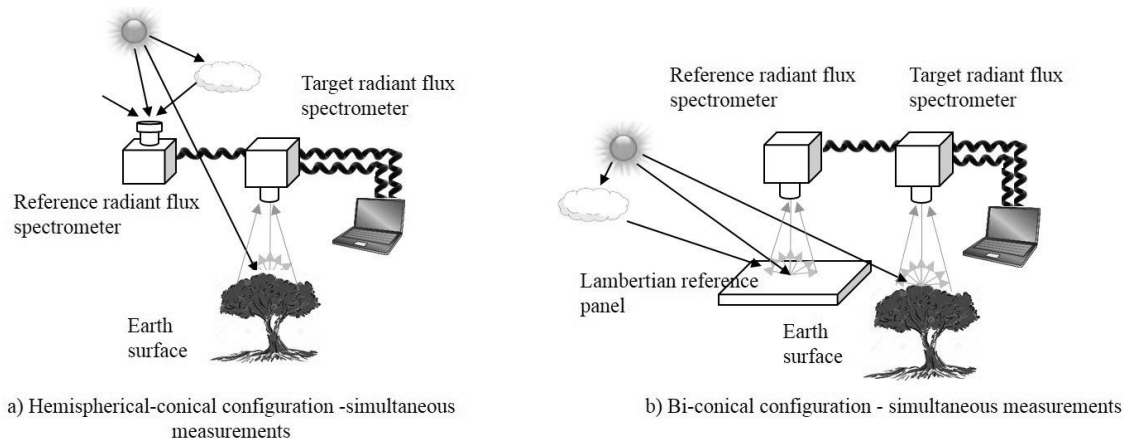


Figure 3. Dual spectrometer dual field-of-view measurement modes

Nevertheless, actually determining of the FOV of field spectrometers has rarely been considered. The manufacturers' specifications for fore optics are generally accepted and used as the delimiting condition. The influence of the light transfer from fore optic to detector and the spectrometers internal optical design are rarely discussed. The complexity of light transfer from fore optic to detector is compounded in full wavelength spectrometer systems as these include multiple detectors with different light paths to each. In these systems the form and positioning of the viewing optics and technology adopted to transfer light from the fore optic to individual detectors may cause significant non-uniformity and discontinuities in of spectral response across the area (the measurement support) from which radiant flux is received. Furthermore, this area may not align with that assumed from the specification provided by the manufacturers for the fore optic. When recording spectra from heterogeneous earth surface targets, it is important to have the area of measurement support be accurately defined as individual reflecting surfaces may be present in varying proportion within this area, as can be observed in Figure 7. And these proportions need to be determined to relate spectral reflectance to state variables or target classifications being considered. The area of measurement support and the spatial and spectral responsivity of an ASD Field Spec Pro FR spectrometer and a SVC GER 3700 spectrometer have been determined by measuring the directional response function (DRF) of each instrument [19]. With an ASD full wavelength system when a lens-based fore optic is used it effectively 'images' the support onto the tip of the fibre bundle. Because the fibres are randomly distributed to three detectors, each detector selective receives light from different areas within the support as each fibre has its own FOV (Figure 4). With the SVC GER3700 design a chromatic aberration is apparent with wavelengths being weighted differently across the FOV and the influence of the slit evident (Figure 5). However, when a bare fibre bundle is used this 'imaging' does not occur (Figure 6) or is a chromatic aberration observed. These results are specific to the spectrometer/fore optic combinations investigated, although similar characteristics can be expected for other instruments/fore optics of these designs and at other measurement distances, the DRFs will vary from those presented

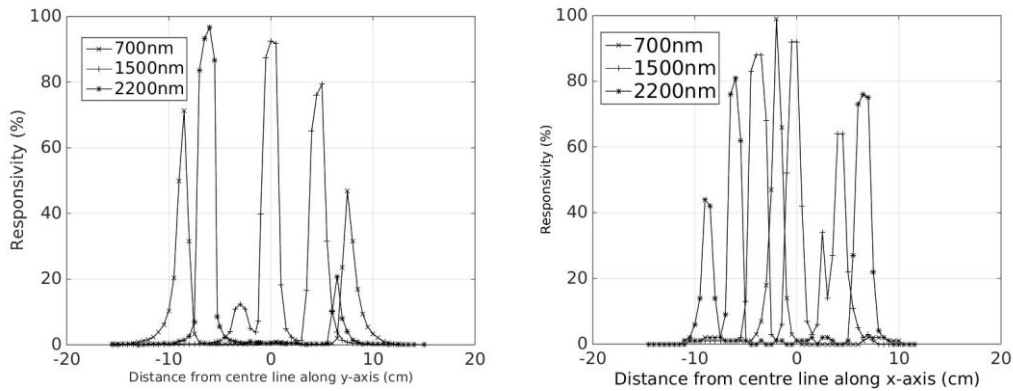


Figure 4. ASD FS with 10deg fore optic DRF across major axes of support showing FOV and response of individual fibres

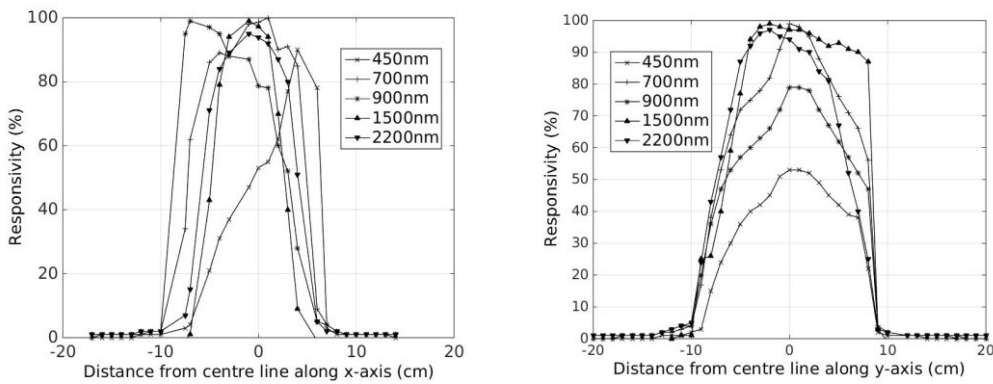


Figure 5. GER 3700 with 10deg fore optic DRF across major axes of support showing chromatic aberration and influence of optical slit

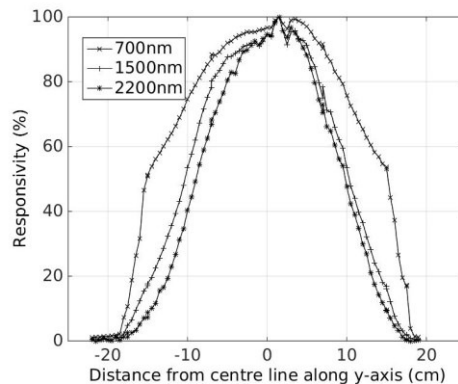


Figure 6. ASD FS with 18deg fore optic (no lens) DRF across major axis of support showing FOV of VNIR fibres constrained by field stop and that the SWIR fibres have a narrower and unconstrained FOV GER 3700 with fibre attachment results similar.

here. The DRFs of these instruments indicate that each reflecting element from which the spectrometer receives radiant flux will be spectrally weighted the integrated measurement recorded in correspondence with its position within the measurement support. The methodology, a fuller discussion of this phenomenon, and recommendation made to spectrometer designers can be found in [19]. It should be noted that ASD now make a fore optic attachment (a ‘scrambler’) and SVC have significantly improved their optical design to minimise these effects. The influence that the DRFs of the field spectrometers has on measurements and on field sampling will now be discussed.

4. EARTH SURFACE SPECTRAL HETEROGENEITY AND FIELD SAMPLING STRATEGIES

To investigate the effect of these erroneous assumptions referred to in the previous section empirically derived DRF data cubes were generated from very high resolution (1 mm pixel) classified 1 m square images of Earth surfaces and spectral profiles of each class placed at each pixel position to generate synthetic data cubes (Figure 7). Five images of each surface type were used to enable statistic validity of the methods to be assessed. These Earth surface data cubes were then convolved with spectrometer DRF data cube generated from the work by [20]. The differences between the spectra generated by this convolution process and those spectra that would have been acquired by the nominal FOV assumed from the manufacturers' specifications are presented. Furthermore, by simulating different field sampling strategies this paper demonstrates the influence of the DRF on measurements and suggests methods of countering the systematic instrument-induced bias.

It was first demonstrated that by rotating the two spectrometer fore optics around their optical centre line the systematic wavelength dependent bias introduced in sampling spectrally heterogeneous Earth surfaces could not be countered. This approach was unsuccessful, even when measurements were made at 1° increments (360 position - which would not be possible in the field due to shading the target surface), as the spectral bias is radially distributed (Figure 8).

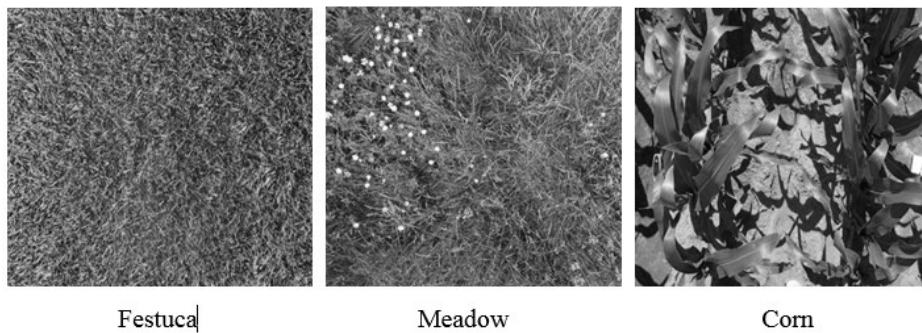


Figure 7. Earth surface images and ecosystem types used to derive synthetic data cubes for modelling studies.

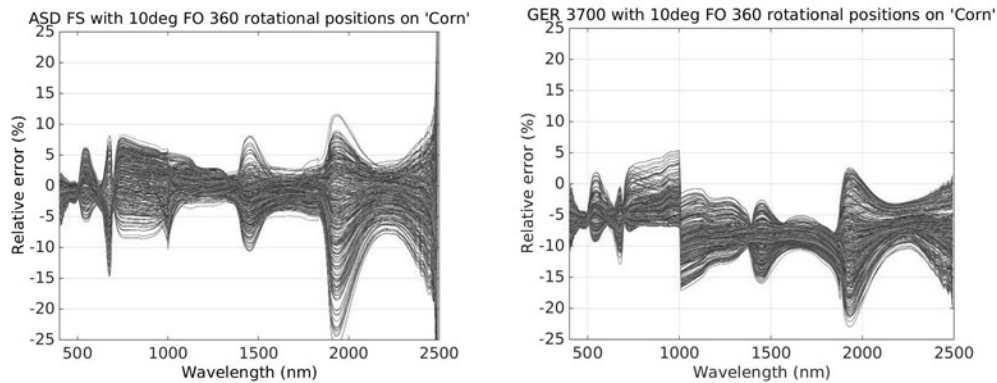


Figure 8. Rotation round optical centre line indicates radial bias as plots are not symmetrical round x-axis.

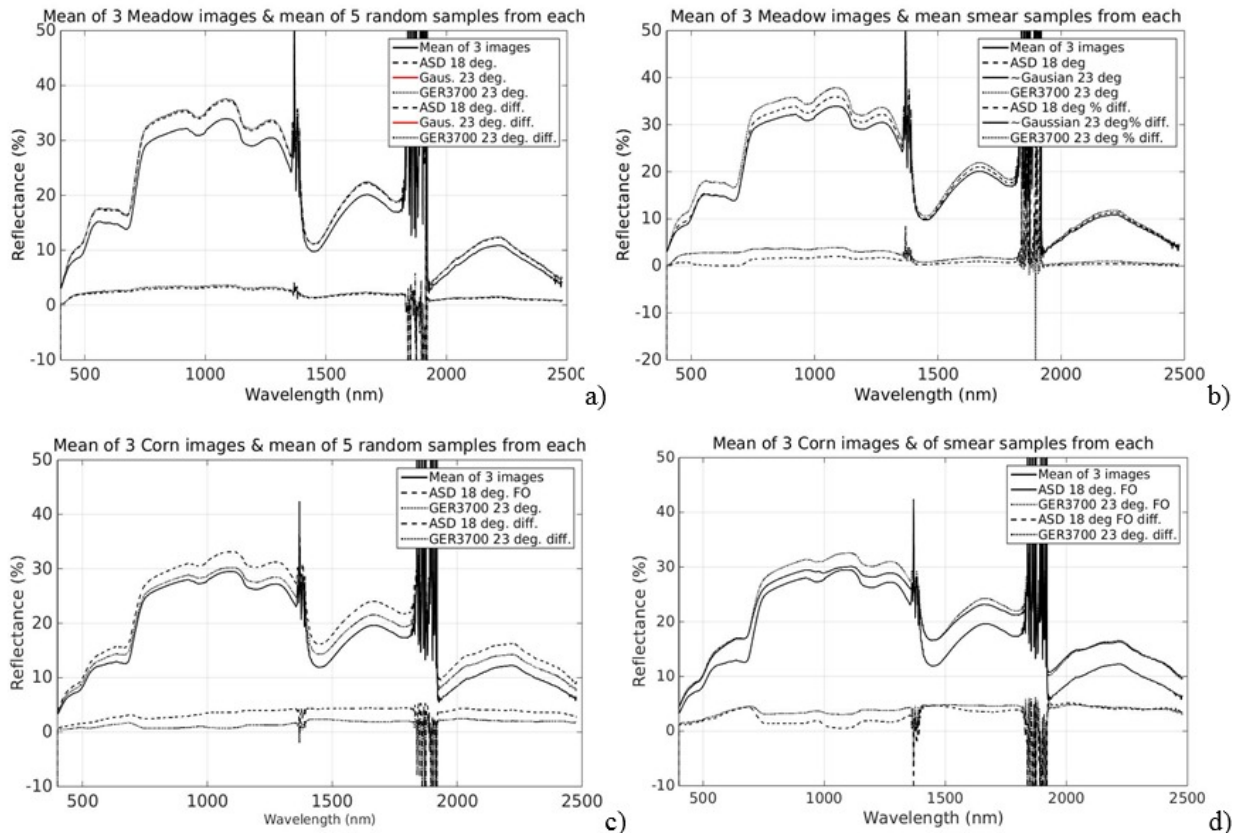


Figure 9a. Random sampling of Meadow images; b) smear sampling of Meadow; c) random sampling of Corn and; b) smear sampling of Corn

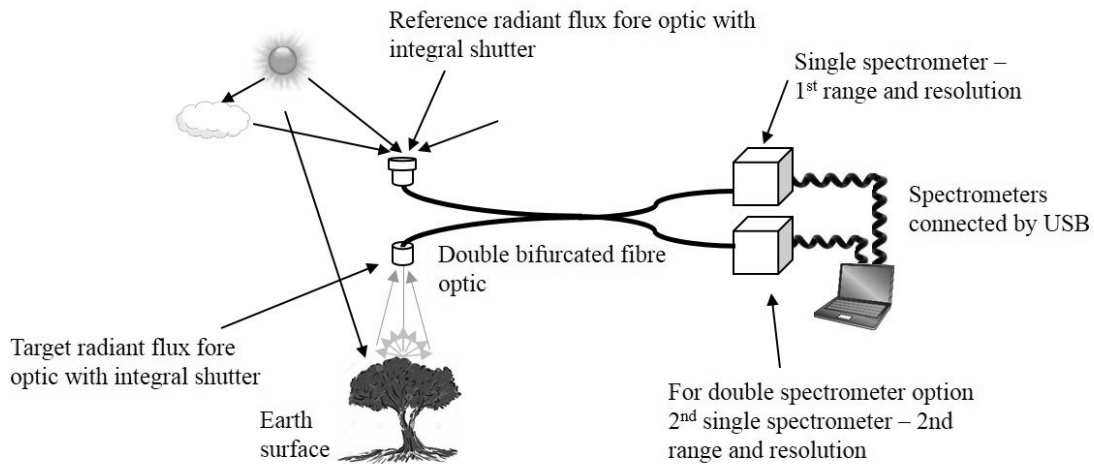
A range of field sampling strategies (transect, random point, and smearing) were then simulated using the same synthetic data/DRF convolution approach. The intention of this work was to determine the most appropriate sampling technique if the intention was to establish relationships between spectral features and state variables physically sampled from the surface using a 1 m square quadrat. All elements within the image would therefore be physically sampled but selectively spectrally sampled by different strategies. The transect technique was considered to be the least appropriate method. This technique, although it may have validity for specific purposes e.g. determining ecological gradients, did not have the statistical validity of the random approach nor the integrated measurement over the larger area of the smear technique and generated the greatest differences. It is therefore not considered further here. The differences between the image means and the simulated spectra generated by both the smear technique and by random sampling, with 5 samples simulated to enable a direct comparison between them, displayed great variability when only one image was considered. However, when the mean of the 3 images was computed and compared to the mean of the sampling techniques each of the 3 images, the maximum difference of approximately 5% was observed for random sampling and approximately 5% for the smear technique (Figure 9a, b, c, and d). However, the results from the smear technique displayed greater spectral variability. When smearing is used in the field normally lengths greater than 1.5 metres are sampled or more than five smears are conducted. Therefore, a more representative mean could be expected, although care has to be taken to smear across rows in the case of corn or an unrepresentative mean may be computed. A fuller discussion of this work is reported in [20].

There is also a need to increase the area over which measurements are integrated for Earth observation (EO) satellite sensor calibration and validation and endmember acquisition purposes so that the near-ground measurement support is of the same order of magnitude as the support for satellite sensor measurements. For EO sensor ground sampling distances of up to 30 metre pixel equivalents are now possible using field spectrometers mounted on sUAVs. In addition, statistically robust random and non-invasive sampling techniques could be implemented as these sUAVs can be programmed to fly to pre-determined way points and the co-ordinates of these could be provided by computed program generated random numbers.

This work is an initial investigation and a greater number of Earth surface types, with a more extensive study, including simulate measurements from UAVs, and rigorous statistical analysis would be required prior to firm recommendations being made. For this work a 5% difference was considered reasonable as this may be comparable with introduced in atmospheric correction processing of hyperspectral images or through general uncertainties (illumination condition variability, for example) and this was used as the threshold criteria.

5. NEW INSTRUMENT AND PLATFORM DEVELOPMENTS

It was evident that with the recent development of miniature single-board computers, micro-electronic modules for wireless communications systems that a spectrometer system could be developed to incorporate commercially available off-the-shelf spectrometer modules (original equipment manufacturer (OEM) optical benches) to produce lower cost and more user friendly spectrometer systems for fixed point logging applications and systems which could readily be mounted at flux sites. The smaller size and reduced power consumption of modern electronics also makes use of spectrometers on sUAVs practical. Python, a programming language familiar to many geoscientists, could be used for both instrument control and data post-processing. A spectrometer system (Piccolo) was subsequently developed and field tested in continuous logging operations during the EUROSPEC Summer School in Sicily during 2014. This system has now been further developed to enable two independent OEM optical benches to be controlled simultaneously. This system (Piccolo Doppio, the measurement mode is displayed in Figure 10 and spectrometer system in Figure 13a) is DFOV with a cosine corrected fore optic to capture down-welling irradiance and the upwelling channel can be configured either for a view angle limited fore optic to capture up-welling radiance or with another cosine corrected receptor to collect hemispherical up-welling radiance. A double bifurcated fibre optic is used to transfer light from the fore optics to the spectrometers therefore each spectrometer receives light from the same Earth surface area (each measurement has the same support). Measurements of grassland reflectance over the visible and near infrared (VNIR) and simultaneous radiant and irradiant flux across the O₂ bands are shown in Figure 11 a) and b), respectively. As the Piccolo Doppio light input is fibre optic-based it can be configured to measure Earth surfaces from any view angle required. Therefore, off-nadir measurements can be made if desired and fore optic could be attached to a robotic arm to 'scan' Earth surface areas in a manner similar to the approach adopted by [21]. Power requirement, physical dimension, weight, spectrometer specification, and software details are listed in Table 1. Data can transmitted by a low-power wireless module radio but also stored on an internal flash memory card to provide data backup. The Piccolo systems can be controlled from a laptop through the wireless connection (an Ethernet connection and a touchscreen tablet interface are currently being developed).



Hemispherical-conical or bi-hemispherical configurations. Near-simultaneous (< 500 milliseconds between) up-welling and down-welling flux measurements

Figure 10. Single or double spectrometer dual field-of-view mode

This system can incorporate up to two USB controlled and fibre-optic input-based OEM optical benches (individual spectrometers without any external optics or software interfaces). This will enable the selection of optical benches with different spectral resolutions and sampling intervals for a diverse range of applications. For example, spectrometers

to measure both reflectance across the visible near infrared region (400 nm to 1,000 nm) and the spectral region which contains the O₂-A and O₂-B band (640 nm to 780 nm) or the SWIR (950 nm to 1,750 nm or to 2,500 nm) regions can be selected. This will enable near-ground measurements of sun-induced fluorescence (SIF) in support of space-based observations and for photosynthesis process model validation and cal/val of satellite-based observation, Sentinel-2 and Sentinel-3 for example.

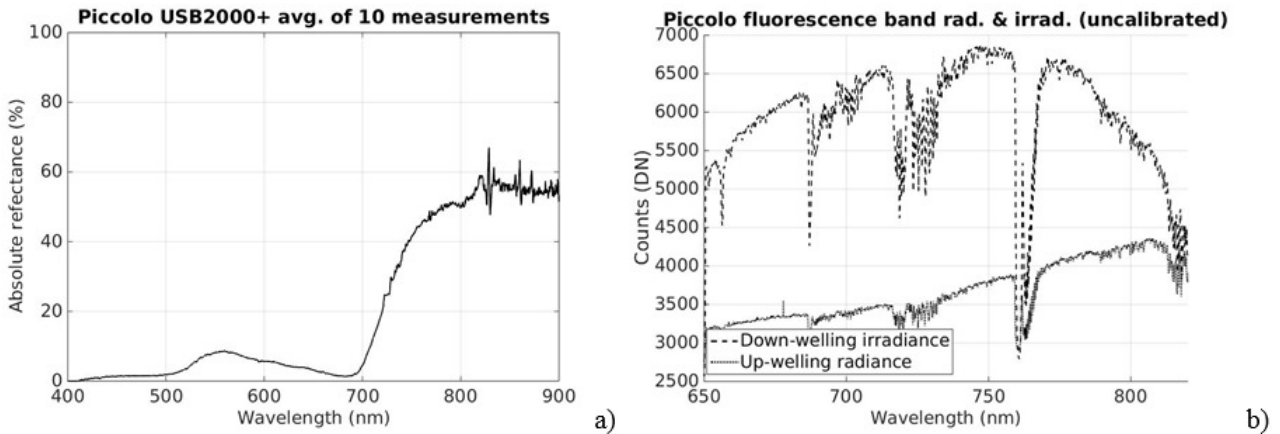


Figure 11a. Piccolo doppio OO USB 2000+ reflectance and b) OO Maya fluorescence bands radiance and irradiance

Table 1. Piccolo Doppio with USB 2000+ QE Pro system power requirements, dimensions and weight

Piccolo Doppio DFOV single or dual spectrometer system		Comment
Operating system/software	Linux/Python	Open source
GUI	Python and Qt	Provided open source
Spectral range considered usable by authors	400nm to 1,000nm and 640nm to 780 nm or 950 nm to 1,750 nm or 2,500 nm	See Ocean Optics specifications
Spectral sampling interval	Dependent on optical bench selection	See Ocean Optics specifications
Spectral band width	Dependent on optical bench selection	See Ocean Optics specifications
Size	120 mm x 120mm x 140 mm	For single spectrometer deployment
	240 mm x 240 nm x 320 mm	For logging with temp. control
Power requirement	<5w (14.8 V lithium polymer battery)	For UAV deployment
	3.5A at +5V (with thermoelectric cooler)	For logging with temp. control
Weight	From 0.8 to 1.9 kg if used with 2 optical benches - one thermoelectrically cooled	For UAV or logging deployment
Single or double bifurcated fibre optic cable length	Max. 5 metres	User selectable. Light weight design available for UAV use

The Piccolo Doppio has now been successfully deployed at fixed point logging locations in forests (Figure 12a) and on a sUAV platform (Figure 13) where it is being used to develop field sampling strategies to support EO cal/val activities by the authors. It has also been deployed on tractor platform and is being tested by Prof. P. Townsend, University of Wisconsin for precision agricultural applications (Figure 14).

6. CONCLUSIONS

A very brief summary of the history of the development of spectroscopy has been presented to indicate its basis in physical optical principles and its providence in Earth observation has been presented. The importance of considering the dynamics of skylight and the importance of having stable conditions to provide the down-welling irradiance measurement to which the up-welling measurement and measurements separated in time and space and by other investigators will be referenced have been highlighted. Uncertainties and errors in the reference measurements should be

quantified and reported as these will propagate through subsequent analysis. The importance of optical design of spectrometers and the characteristics of each instruments DRF should be considered when selecting instrument for field work and the purpose of this work – biophysical estimation, cal/val activities, etc. will need to be considered as will the different approaches to field sampling. It should be borne in mind the humans unaided by technology do not do ‘random’ sampling well. Humans are intuitively attracted visual highlights or inconsistencies negating the statistical validity of our measurements and sampling strategy. Investigators need to generate tables of random numbers, randomly assign GPS locations to these and sample spectrally at these point to validly use the power of statistic in their work. Finally the development of on spectrometer system to improve the utility of field spectroscopy and enable affordable small unmanned aerial vehicles to be used as platform has been presented. These last two developments will enable near-ground Earth observations to be made with the same support as space-based observations for the first time. This will then enable uncertainties and errors associated with ground reflectance products derived from atmospheric correction of the space-based observations to be better quantified.

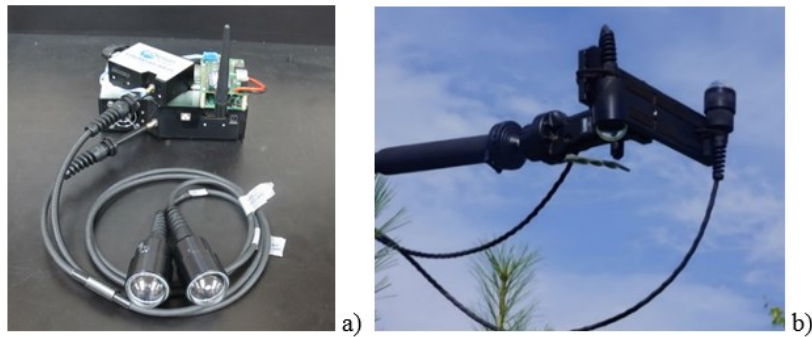


Figure 12a. Piccolo Doppio dual optical bench DFOV spectrometer system and b) mounted at a fixed location in a forest

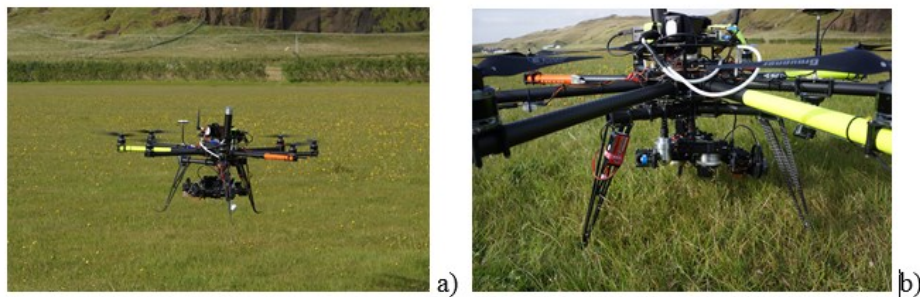


Figure 13a Piccolo USB 2000+ irradiance FO on top of sUAV and b) FOV fore optic on gimbal below sUAV



Figure 14a. Piccolo Doppio with OO USB 2000+ and NIRQuest on tractor and b) Up- and down-welling fore optics on gimbal. Photos provided by A. Singh, U. of Wisconsin)

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