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Citation for published version:

MacArthur, A, Robinson, I, Rossini, M, Davis, N & MacDonald, K 2014, A dual-field-of-view spectrometer system for reflectance and fluorescence measurements (Piccolo Doppio) and correction of etaloning. in *Proceedings of the Fifth International Workshop on Remote Sensing of Vegetation Fluorescence*. European Space Agency, Fifth International Workshop on Remote Sensing of Vegetation Fluorescence, Paris, United Kingdom, 22/04/14. <<http://www.congrexprojects.com/2014-events/14c04/proceedings>>

Link:

[Link to publication record in Edinburgh Research Explorer](#)

Document Version:

Publisher's PDF, also known as Version of record

Published In:

Proceedings of the Fifth International Workshop on Remote Sensing of Vegetation Fluorescence

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A DUAL-FIELD-OF-VIEW SPECTROMETER SYSTEM FOR REFLECTANCE AND FLUORESCENCE MEASUREMENTS (PICCOLO DOPPIO) AND CORRECTION OF ETALONING

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ABSTRACT

A lightweight, wirelessly controlled or autonomous, dual-field-of-view spectrometer system for environmental monitoring from rotary-wing unmanned aerial vehicles or for fixed deployment on masts at research sites has been developed. This system can incorporate up to two USB controlled and fibre-optic based spectrometers. This will enable the selection of spectrometers 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 and the O₂-A and O₂-B spectral regions can be incorporated. This will advance the near-ground measurement of sun-induced fluorescence in support of space-based observations and for photosynthesis process model validation. A new high performance spectrometer from Ocean Optics, the QE Pro, can be used with this system. However, as the QE Pro has a back-thinned detector, it suffers from etaloning to some degree. To enable the use of the QE Pro to determine sun-induced fluorescence requires that this etaloning be corrected. The linearity of the QE Pro and nature of etaloning displayed have been investigated. Two methods to correct etaloning were then tested and the results presented here and recommendations made.

1. INTRODUCTION

Research to improve estimates of the Earth surface/atmosphere carbon dioxide (CO₂) exchange through photosynthesis requires information of the physiological state of vegetation. Measurements of sun-induced chlorophyll fluorescence (SIF) have potential for the assessment of actual plant photosynthesis from space and only recently measurements of SIF from airborne and satellite platforms have been proven to be feasible [1]. However, corresponding near ground measurements are required to validate these SIF estimates since the correction for atmospheric effects plays a major role in SIF estimation from air- and spaceborne measurements [2]. Near ground measurements are also required to assess the sensitivity

of SIF to changes in photosynthetic activity at spatial (leaf and canopy) and temporal scales, scales at which biogeochemical processes and ecosystem functional properties are already being assessed by other means in carbon flux observation networks [3]. Very high spectral resolution spectrometers are currently available that measure across the spectral region containing the O₂-A and O₂-B bands, where SIF estimation is possible, and other spectrometers are available for measuring across the wider visible-near infrared region, used to determine indices such as the Photochemical Reflectance Index, an alternative indicator of photosynthetic activity. However, the very high spectral resolution systems used to date often have poor signal to noise and low sensitivity, requiring measurements to be made at different integration times for each O₂ band. In addition, current methods either rely on sequential measurements of a reference standard (to estimate solar irradiance) and the target Earth surface, both using a restricted field-of-view (FOV) fore optic, or sequential measurements of upwelling radiance and downwelling irradiance using a cosine corrected fore optic with a hemispherical FOV. With both these approaches there are time delays (at best multiple seconds) between measuring downwelling and upwelling radiances. These delays add to measurement uncertainties due to changes in sky conditions between the individual measurements, particularly in northern Europe. Furthermore, the current systems, while possibly suitable for fixed location deployment and high frequency temporal measurements, are not designed, and would be impractical to use, to capture the spatial variability necessary to spectrally characterise the 'foot print' of carbon flux observation systems.

A design and the preliminary laboratory performance characteristics of a light weight dual-field-of-view spectrometer system for the near simultaneous measurement of both reflectance and SIF are presented here. This system utilises a double bifurcated fibre optic incorporating a novel switching mechanism such that it enables reflectance and SIF to be measured simultaneously from the same Earth surface area and

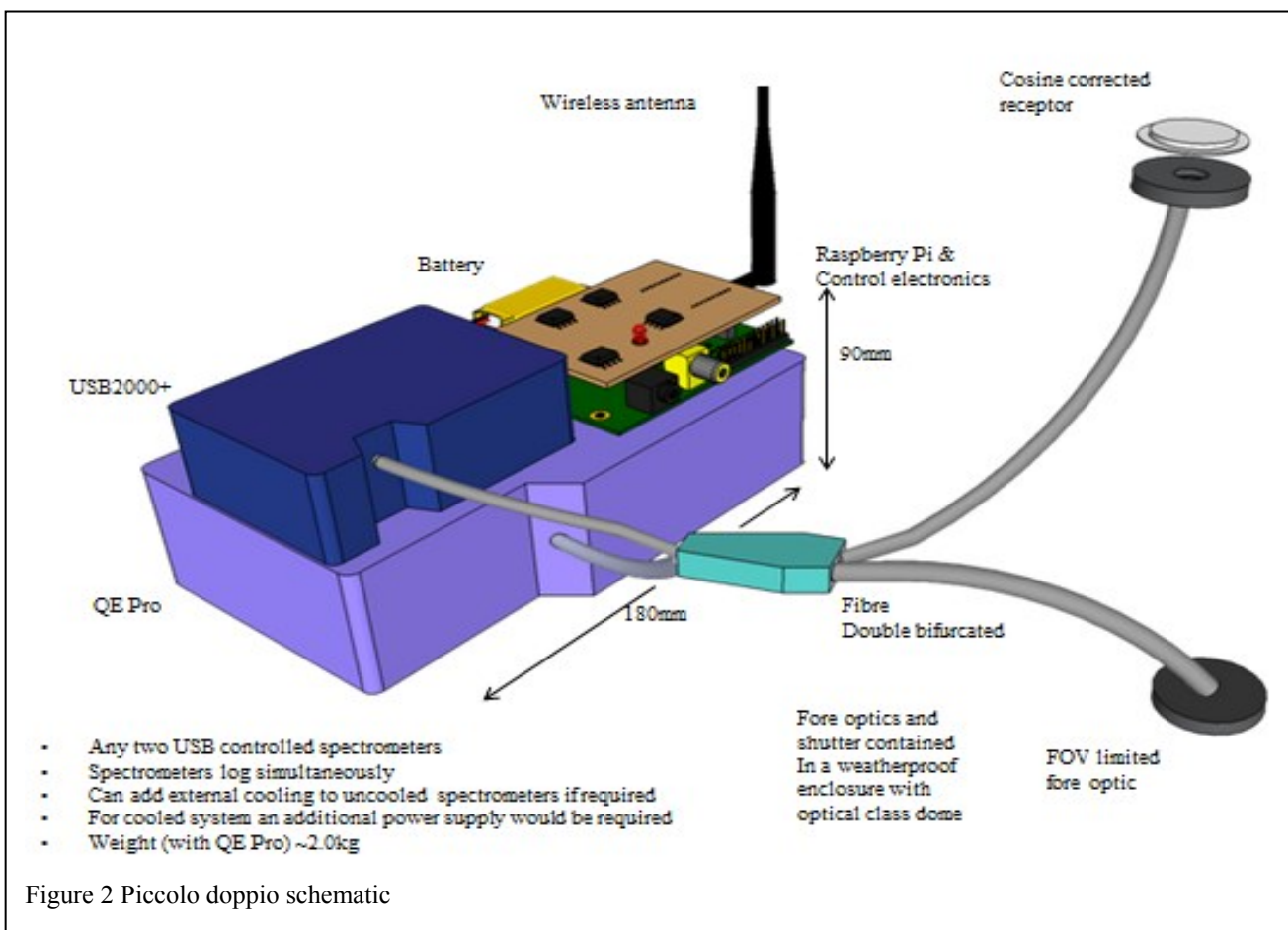
target and reference irradiance to be measured at frequencies greater than 5Hz. This system is light weight, self-contained, and wirelessly controlled to enable it to be deployed on rotary-wing unmanned aerial vehicles (UAVs), as well as being able to be used for fixed location high temporal frequency logging measurement approaches. It can also contain the latest very high radiometric resolution Ocean Optics QE Pro optical bench which may enable both O₂ bands to be measured simultaneously and with the same integration time.

2. INSTRUMENT DISCRIPTION

During the course of COST Action ES0903 “Eurospect” [4], the UK Natural Environment Research Council Field Spectroscopy Facility, based in the School of Geoscience, University of Edinburgh, identified the need for a light weight spectrometer system for deployment on rotary-wing UAVs to enable measurements to be made in the spatial domain and capture the spectral heterogeneity of surfaces within flux tower footprints. In addition, it was evident that with the recent development of single-board computers (e.g. Raspberry Pi), micro-controllers (e.g. Arduino), and micro-modules for wireless communications (e.g. Xbee using the ZigBee networking standard) systems

could be developed for spectrometer modules to produce simpler and more user friendly spectrometer systems for fixed point logging applications and systems which could readily be mounted at flux sites. In addition, the Raspberry Pi’s native software is Python which is open source and gaining wide use for instrument control and data post processing.

A spectrometer system (Piccolo) measuring across the 400 nm to 1,000 nm (VNIR) spectral range was developed and field tested for continuous logging operations during the EUROSPEC Summer School in Sicily during 2014. This system has now been further developed to enable two independent optical benches to be controlled simultaneously. This system (Piccolo doppio) is dual-field-of-view 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 (Fig. 1). A double bifurcated fibre optic is used to transfer light form the fore optics to the spectrometers therefore each spectrometer receives light from the same Earth surface area (each measurement has the same support). As the Piccolo doppio is fibre optic based it can be configured



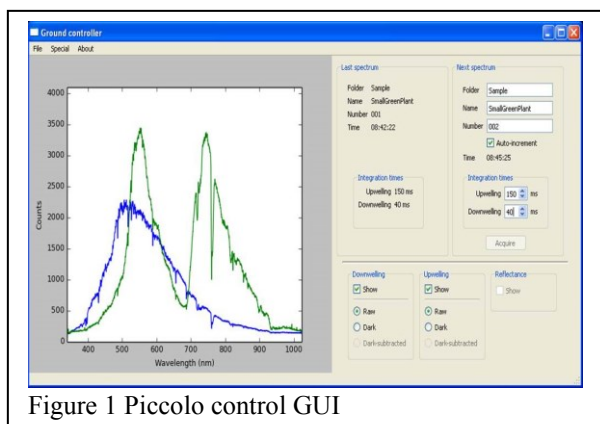


Figure 1 Piccolo control GUI

to measure 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 if required, in a manner similar to the approach adopted by [5]. The Piccolo doppio spectrometer system is contained within an IP63 'all weather' enclosure. The system can be powered: by a lithium polymer battery, for UAV deployment; from a flux tower's main power supply; or from dedicated solar panels for long term deployment. Power requirement, physical dimension, weight, spectrometer specification, and software details are listed in Table 1. Data is transmitted by a low-power (ZigBee) radio but also stored on an internal flash memory card to provide data backup. The spectrometer system can be controlled from a laptop through the wireless connection, and the GUI is displayed in Fig. 2, or from an executable installed on a PDA.

3. SPECTROMETER OPTIONS

The Piccolo doppio is designed to be able to be used with any two fibre optic based and USB controlled spectrometer optical benches but also has a serial control communication interface. For SIF measurement the spectrometer optical benches considered are the Ocean Optics USB2000+ to measure the 400 nm to 1,000 nm spectral range from which the photochemical reflectance index can be determined and one of the other spectrometers listed in Table 2 to measure across a narrower (640 nm to 840 nm or 640nm to 800 nm) spectral range at higher sampling interval and narrower band widths to measure across the O₂-A and O₂-B bands.

To date the Piccolo doppio has been successfully tested with the Ocean Optics USB2000+ and the HR4000 optical benches. However, trials with the Maya and QE Pro spectrometers have been delay as etaloning was evident in the test spectra. Etaloning has been reported in the previous generation of the Ocean Optics QE spectrometer series and concerns expressed by the Earth observation community that this would prohibit their use to measure SIF due to the very high specification

requirements to determine this parameter and because of differences between the light source used in laboratories for calibration and characterization (tungsten halogen with a colour temperature of say 3,200 K) passive source, the sun (with a colour temperature of say 6,000 K), used for optical remote sensing in the field.

4. ETALONING

To achieve high conversion efficiency and sensitivity, and hence, with a suitable analogue to digital converter, high digitization (the QE Pro is 18-bit) back-thinned charged coupled device thermo-electrically cooled detectors are used. However, due to their reduced thickness these detectors may not absorb all incident near infrared (NIR) radiation. Back-thinned CCDs become semitransparent in the NIR region of the spectrum and form a resonant optical cavity in which wavelengths which fit an exact integer number of times between the surfaces bounce back and forth between the CCDs internal surfaces and are sustained in it to form constructive and destructive interference patterns typically at 5 nm intervals [6]. As not all light is incident normal to the CCD surface these reflections travel along the CCD and cause the characteristic ripple seen in the NIR regions of the spectra measured. As etaloning is a function of the NIR wavelength and the thickness of the CCD the wavelength at which it becomes evident will depend on the thickness of the CCD. Etaloning will therefore be spectrometer specific. Nevertheless, as etaloning is a function of the wavelength of the NIR light and the thickness of the CCD, it is hypothesised that it can be corrected in post processing and enable these spectrometers to be used for SIF measurements.

5. CORRECTING ETALONING

To be able to correct etaloning in post processing it first has to be demonstrated that it is linear with respect to intensity of light. Then it is necessary to demonstrate that it is stationary in respect to wavelength. The QE Pro #00114 held by the NERC Field Spectroscopy Facility at the University of Edinburgh was used to determine if etaloning could be corrected in post processing.

A Hoffman 6" diameter radiance integrating sphere with tungsten halogen lamp and electronic control (accuracy of 1 fl with an uncertainty $\pm 0.1\%$) was used to generate light at 20 different levels of intensity, from 50 fl to 1,000 fl, at each of two temperature settings, -10°C and -20°C , and 30 measurements were made at each setting. The spectrometer's averaging was set to 30, electronic dark current was automatically subtracted, and the Ocean Optics non-linearity correction was enabled. The QE Pro spectrometer's response to different intensities of light is not linear, as are all CCD detectors, although the linearity of each pixel in the array is claimed to be

identical [7]. Ocean Optics address this non-linearity by fitting a 7th order polynomial to 9 pixel values across the array during the laboratory calibration process. Non-

linearity correction coefficients can then be computed for each pixel and applied to the measurements obtained, if this option is selected while

Table 1. QE Pro power requirements, dimensions and weight

Piccolo Doppio light-weight compact DFOV VNIR spectrometer system		Comment
Operating system/software	Linux/Python	Open source
GUI	Python and Qt	Provided open source
Spectral range	400nm to 1,000nm and 650nm to 800nm (1,000nm to 1,700nm option in development)	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 nm x 240 nm x 320 nm	For logging with temp. control
Power requirement	<5w (14.8 V lithium polymer battery)	For UAV deployment
	3.5A at +5V (with TE Cooler)	For logging with temp. control
Weight	Up to 1.9 kg if used with thermoelectrically cooled spectrometers	For UAV or logging deployment
Fibre length	Max. 5 metres	User selectable. Light weight design available for UAV use

Table 2 FSF Ocean Optics spectrometer configurations

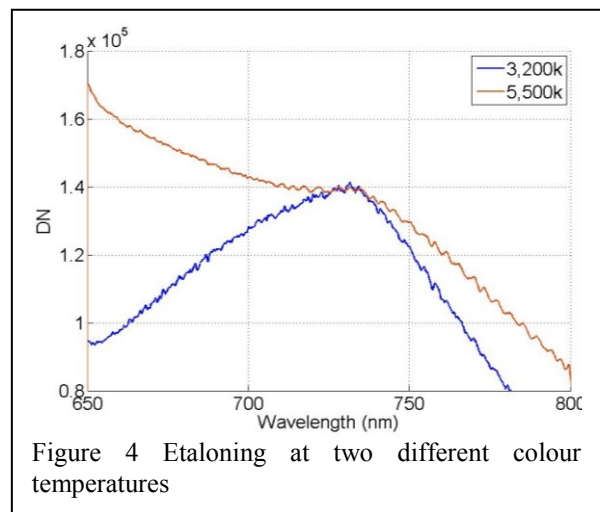
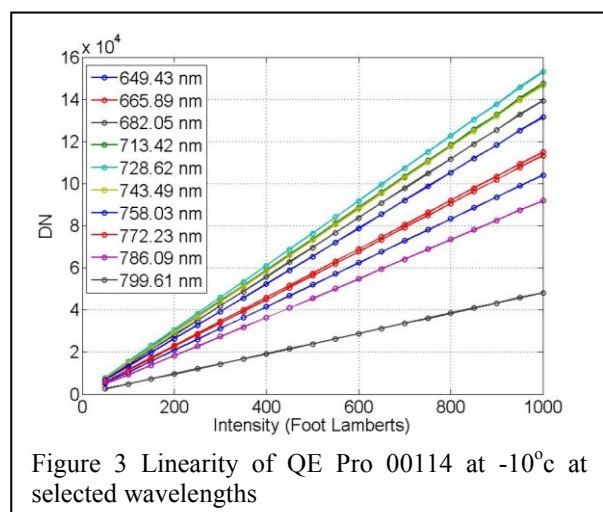
	USB2000+	HR4000	Maya	QE Pro
Optical slit	25 μ m	25 μ m	10 μ m	10 μ m
Spectral range*	400 nm to 950 nm	~650 nm to 840nm	~650 nm to 840nm	~650 nm to 800nm
Sampling interval		~ 0.05nm	~ 0.1nm	~ 0.1nm
FWHM		~0.21nm	~0.31nm	~0.31nm
Digitisation		16-bit	16-bit	18-bit

*This is the spectral range considered usable by FSF

setting the spectrometer measurement configuration parameters or can be corrected in post processing.

For this experiment, automatic non-linearity correction was selected; the spectrometer's integration time was set to achieve approximately 160,000 digital counts at

1,000fl, close to Ocean Optics' automatic integration maximum setting of 85% of 180,000 counts [7]. It is acknowledged that it is not possible to de-convolve etaloning linearity and detector linearity by this method. Nevertheless, it is the system's linearity that is key to making accurate measurements and it is the system's it



that is being tested in this work.

When the spectrometer's measured response at each level of intensity is plotted (Fig. 3) for a selection of wavelengths, it can be seen that the response, after application of Ocean Optics' non-linearity correction, it seems to be linear. However, a root mean squared error of, on average, 140 counts was noted and the non-linearity corrected pixel values were all within 200 counts of the linear model. Therefore, there is some minor deviation from linearity measured. This was found to be the case at both -10°C and -20°C, although for brevity only data at -10°C are presented. Ocean Optics CCD are shallow well devices and rely on multiple measurements being made and averaged. Therefore, the spectrometer's linearity (after corrections) can be considered to be reasonable and may be sufficient to comply with the hypothesis' first condition, that the spectrometer's response is linear with respect to intensity, to enable correction of etaloning by post processing is met.

5.2 Etaloning stationarity with respect to wavelength

An Ocean Optics HL-2000 adjustable light source with a tungsten halogen lamp and a colour temperature of approximately 3,200k was used and thirty measurements made again with an average of 30, electronic dark current subtracted, and non-linearity correction enabled. A dichroic colour correction filter (Comar 01 1A 25) was then used to adjust the colour temperature of the lamp from approximately 3,200k to approximately 5,500k and thirty measurements again made. The mean spectra in raw digital counts (DN) of each of these measurements are displayed in Fig. 4. A smoothing spline was then fit to each of these spectral profiles and the residuals (the difference between the fit and the data) calculated. These residuals are displayed in Fig.5

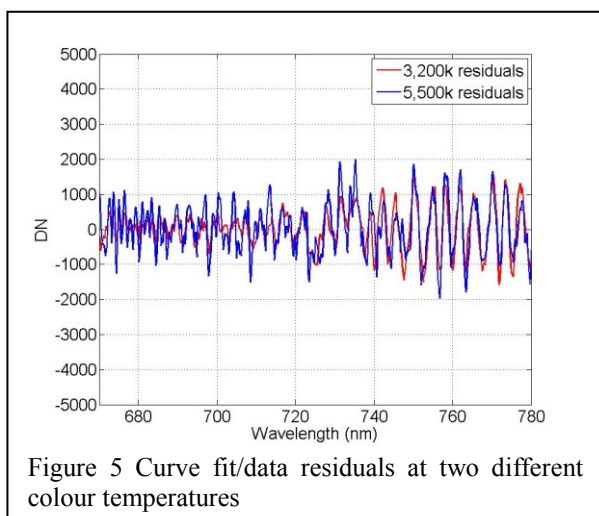


Figure 5 Curve fit/data residuals at two different colour temperatures

From Fig. 5 it is evident that etaloning is stationary with regard to wavelength for different levels of intensity (at different DN per wavelength interval) and source colour temperature, as the constructive and destructive interference etalon patterns align for each of the spectral measurements. It should be noted that due to the curve fitting approach the useful spectral range is reduced from 650 nm to 800 nm to 670 nm to 780 nm. However, this still covers both O₂ bands. It can also be noted from Fig. 5 that the maximum difference between the spectra for each colour temperature at any wavelength interval is less than 100 digital counts at 720 nm which represents less than 0.7% of the dynamic range of the measurement at that wavelength. The differences at other wavelengths are of the same order and this is a lower order of magnitude than laboratory calibration uncertainties [9].

5.3 Correction of etaloning by referencing

As etaloning has been demonstrated to be reasonably linear and stationary, two approaches can be considered to correct this phenomenon in post processing. The first is called the 'referencing' method. This requires a calibrated laboratory light source (Fig. 6a) and spectral measurements are made of this source (Fig. 6b). Then the difference between these and the known output of the source computed (Fig. 6c) and correction factors per wavelength interval ascertained. Mathematically this is presented in Eq. 1 with wavelength omitted for clarity. The instrument response function per wavelength interval is then convolved with each spectral measurement to generate the etalon corrected spectra.

$$\text{Inst. Response} = \frac{\text{measured spectrum (DN)}}{\text{black body (or source cal. file)}} \quad (1)$$

This procedure was followed and the Instrument Response coefficients shown in Fig 6c we determined. Note QE Pro acquisition parameters were again set to achieve a maximum count of 160,000, averaging 30, electronic dark subtracted and non-linearity enabled. Measurements of the tungsten halogen source were then taken at 20 different levels of intensity and 'corrected' by applying the instrument's response function. The resultant spectra are displayed in Fig. 7.

However, it is evident from Fig 7 that some 'noise' is present in all the spectra other than the one used to generate the instrument response function (the highest spectrum), although when examined in detail the variation was less than $\pm 0.7\%$. This could be due to the slight non-linearity of response identified in the linearity check discussed in the previous section. An alternative approach to correction of etaloning which may better account for this slight non-linearity was tested subsequently.

5.4 Correction of etaloning by curve fitting and residual interpolation

To try to better account for this slight non-linearity and not rely on a calibrated light source, the Ocean Optics HL-2000 adjustable tungsten halogen source

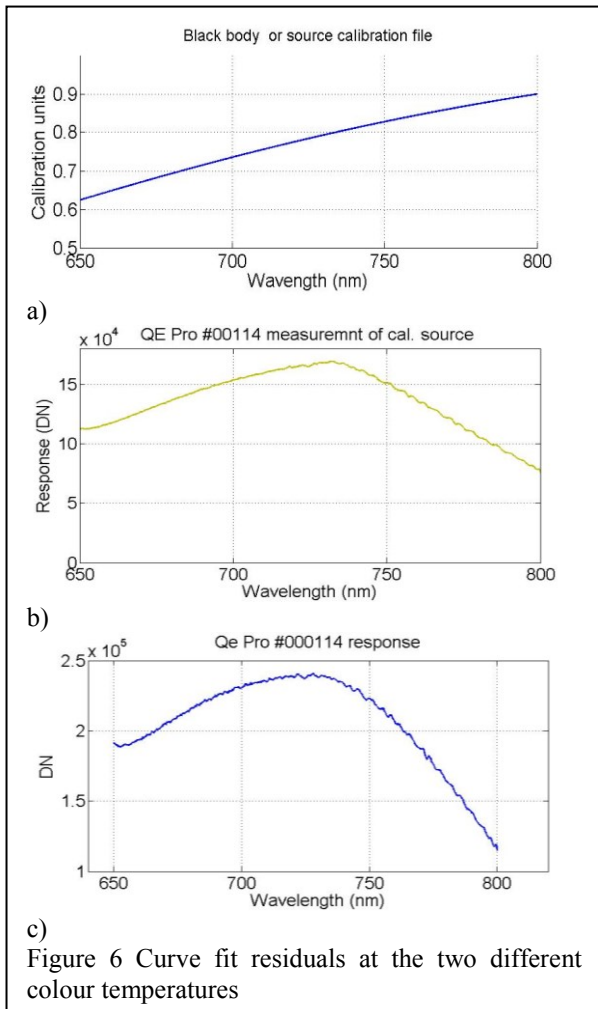


Figure 6 Curve fit residuals at the two different colour temperatures

was again used. The QE Pro was set: to average 30 measurements; integration time to achieve 160,000 counts, dark current subtracted; and non-linearity correction enabled. Measurements of the source made at 20 levels of intensity. Three of these were selected to assess the method and the remaining 17 used to develop the correction method.

Matlab software was used to fit a smoothing spline with a factor of 0.99 to each of the 17 spectra measured. Examples of two of these spectral measurements and the corresponding smoothing spline fits are shown in Fig. 8, with the spectral range truncated to enable details to be seen. The residuals (the differences between the measurements and the smoothing spline model fits) were then calculated for each wavelength interval of each spectral measurement. This provided an array of correction coefficients per wavelength interval for each DN

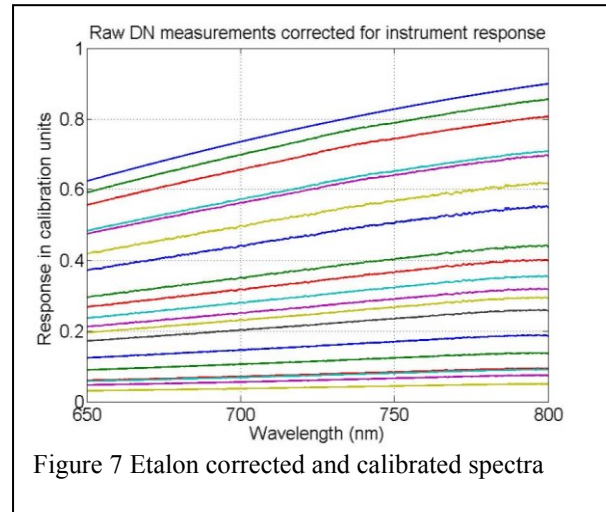


Figure 7 Etalon corrected and calibrated spectra

measured. Note as the nonlinearity correction converts the measured DN integer to floating point precision these values needed to be transformed back to integers by 'rounding' prior to using as correction coefficients. To enable etaloning to be corrected in post processing and at levels of light intensity not measured here, these residuals were linearly interpolated for each possible DN integer value between 0 and 160,000. This was repeated for each wavelength interval and resulted in a 160,000 x 1044 array of correction coefficients (1044 is the number of wavelength sampling intervals in the QE Pro used for this work). Note this array was then truncated to the spectral range 660 nm to 780 nm as the curve fitting technique does not produce reliable results towards the extremes of the data. This truncated array (160,000 x 800) is then used as a look-up table of coefficients for etalon correction. It contains a coefficient for each possible DN value that could possibly be measured and at each wavelength interval across the 660 nm to 780 nm spectral range. When any spectral measurement is now made an etaloning correction coefficient can be found by

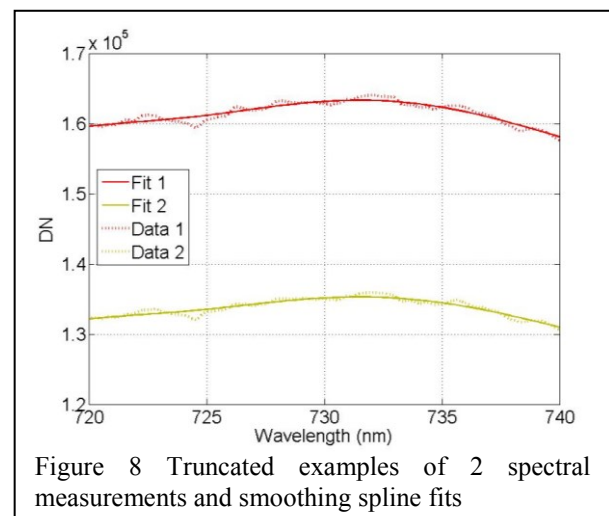


Figure 8 Truncated examples of 2 spectral measurements and smoothing spline fits

using the DN value and wavelength interval to index into the correction coefficient look-up table. Then the appropriate correction coefficient can be added to the measured data and a spectrum corrected for etaloning, including any minor deviations from spectrometers linearity, generated.

To test this correction process, the three spectra not used to generate the look-up table were used. When the appropriate residuals from the look-up table were added to these test data the spectra shown in Fig. 9 were generated. As can be seen in this figure the etaloning has been corrected and a 'smooth' spectrum produced. Two of these corrected spectra are shown with the original spectra in detail Fig. 10 and the effects of the correction can be seen.

To quantitatively assess how well this curve fitting and residual interpolation method had corrected etaloning, a smoothing spline with factor 0.99 was fitted to these three spectra following the procedure used to generate the residuals. When these smoothed spectra were compared with the etalon corrected spectra a maximum difference of 10 counts was noted between each at any of the

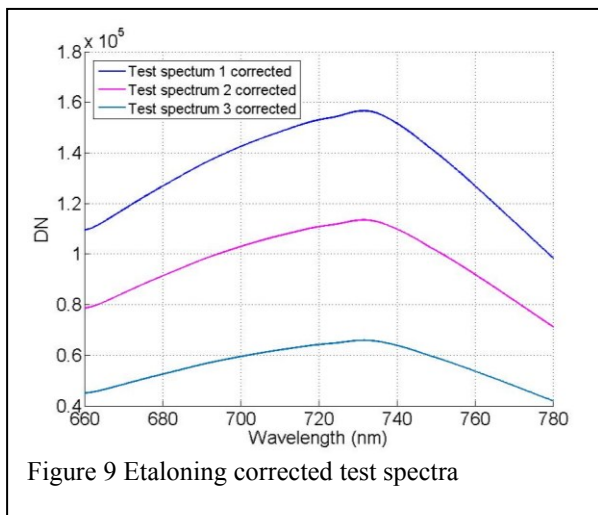


Figure 9 Etaloning corrected test spectra

wavelength interval. This confirms that this curve fitting, residual interpolation and look-up table correction process achieves a significantly more accurate correction of etaloning than was achieved using the 'referencing' approach. It also demonstrates that QE Pro spectrometer etaloning can be successfully corrected in a post processing procedure.

5.5 Correction of etaloning for measurements acquired under natural illumination

For this post processing correction method to be applied to data acquired in the field under natural illumination, it will be necessary to increase the dynamic range measured (to generate the residuals)

towards either end of the spectrometers spectral range as can be seen for the 3,200 K spectrum in Fig. 4 as the data cannot be reliably extrapolated beyond the maximum measured in the look-up table generation process for any wavelength interval. To achieve this, a lamp fitted with filters to change the colour temperature to that close to the colour temperature of the sun or blocking filters, to avoid the detector saturating in the region where it is most sensitive (around 740 nm in the case of QE Pro #00114) will need to be used.

6. CONCLUSION

A light weight DFOV spectrometer system (Piccolo doppio) has been described which can control up to two USB and fibre optic based spectrometer optical benches. Spectrometers such as the Ocean Optics USB2000+ series, HR4000 series, Maya series and QE Pro series can be used. The QE Pro in particular offers a step-change in spectrometer dynamic range which will be of great benefit in SIF measurements. As the Piccolo doppio measures upwelling radiance (and downwelling irradiance) through the same fibre optic based fore optic and at the same sampling interval and full width half maximum bandwidth, the uncertainties in field

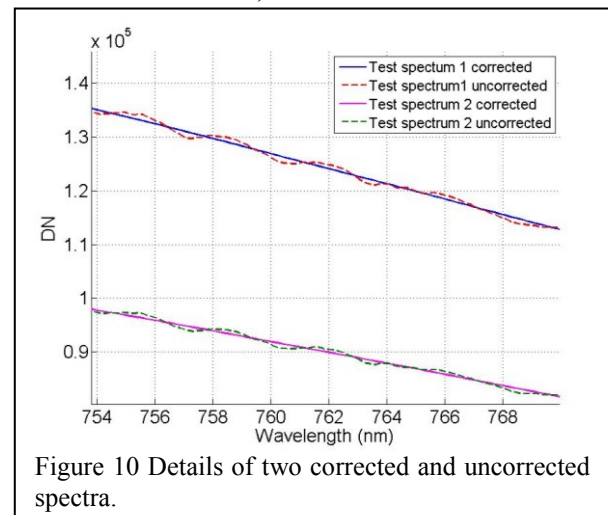


Figure 10 Details of two corrected and uncorrected spectra.

spectroscopic measurement highlighted by [8] are minimised. In addition, as this spectrometer can be mounted on UAV platforms or used for fixed point applications, the same instrument can be used to measure at both the high temporal frequencies required for logging applications at flux tower sites and to sample in the spatial domain across flux tower foot prints. Field trials of FSF system with USB2000+ and QE Pro will begin during the summer of 2014.

A photon's energy does not change with the color temperature of the light source it is only the flux density at that energy level that varies. Therefore, the color temperature of the source, albeit the sun or a laboratory tungsten halogen lamp, does not change the nature of

etaloning displayed by a particular spectrometer. Nevertheless, the incident angle of light onto the CCD must not change or it will affect the etaloning displayed. A fibre optic light input accessory directly attached to the spectrometer is therefore recommended. In addition, it was noted during this work that the QE Pro spectrometer displayed a different level of responsivity at each of two temperature settings used (-10°C and -20°C), although there was no change in etaloning stationary with respect to wavelength evident between these two temperature settings. Therefore, it is recommended that the same temperature setting be used for both etalon correction data acquisition and field measurements. It is strongly recommended that the QE Pro detector cooling be used to ensure stability. It also needs to be borne in mind that the QE Pro is a shallow well device. Consequently, a significant degree of the accuracy and precision achieved is dependent on multiple measurements being made and these averaged to produce representative mean spectrum.

Finally, it has been demonstrated in this work that etaloning in back-thinned CCDs appears to be stationary and that data acquired with the QE Pro spectrometer, with non-linearity correction enabled, is reasonably linear. Consequently, etaloning can be corrected to in post processing to within $\pm 0.7\%$ by using the 'referencing' approach and to within 10 counts when the curve fitting and residual interpolation approach is used. The 'referencing' approach would need to be used in fluorescence measurement applications where absolute values in SI units are required as the light source would be calibrated. The 'curve fitting and residual interpolation' approach would then be better suited to fluorescence relative measurement approaches such as those which use O₂ band infill assessment where very small changes in signal need to be measured. Further work will now be undertaken to generate a look-up table for correction of the full dynamic range of the QE Pro at each of the usable wavelength sampling intervals.

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