Mark One Lifestyle, Inc.

A Study of StellarNet Silver Nova Spectrometer

Data Collection

- Date: 2015-04-17
- Ticket: as-302
- Git Repo: data.mkone.co/var/git/science/vessyl/as-293.git

- Git Branch: master

Analysis

- Ticket: va-94
- Git Repo: git@git.mkone.co:vessyl-algorithms/algorithms.git
- Git Branch: va-94

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Revision Control

Revision Number	Revision Date	Notes	Owner
1.0.0	2015-04-22	First draft release	Ehson Ghandehari

Introduction

It is critical to create a spectroscopic database for 500 drinks. This database particularly will be a valuable source for: 1) storing fingerprint spectroscopic-response of commercial drinks, and 2) being utilized to identify the most optimum LED set to be installed in the Halo Vessyl. Therefore, preparing a Golden Setup (GS) for spectroscopic data collection is necessary. The GS should be capable of providing high-resolution spectra in 250-1100 nm wavelength range. In other words, covering the Ultra Violet (UV: 200-400 nm), visible (400-800), and Near Infra Red (NIR>800 nm). The spectroscopic data in NIR region may provide valuable information about chemical bonds of liquid. Therefore, selecting a spectrometer capable of collecting reasonable intensity in NIR is essential. The science and Algorithm team at MarkOne reported that the current USB4000 and HR4000 spectrometers (Ocean Optics, Dunedin, FL, USA) were not capable of collecting high-integrity signals in NIR region. A Silver Nova spectrometer (S/N: 15033104) (StellarNet, Tampa, FL, USA), was tested as a possible alernate spectrometer. Based on the report **(va-85)** and communications with vendor, it was concluded that the spectrometer was a defected unit. A new Silver Nova spectrometer (S/N: 15040704) had been replaced. The pupose of this report is study the functionality of spectrometer for data collection.

Methods

The data was collected in transreflectance mode. Prior to any measurement, the Deuterium and Halogen light bulbs were left on for at least 15 min to stabilize the lightsource. The data was collected based on AS-292. Briefly, the white measurement was 128 scans (1 trial) of distilled water with opened shutter, and the dark measurement was a trail with closed shutter. The measurements were taken at different integration times: a) from 20 ms to 200 ms by increments of 20 ms. b) from 200-1000 ms by increaments of 100 ms.

Setup

The setup used in the data collection was the red golden setup. The red golden setup consisted of a light source (Ocean Optics DH-2000; serial number 005400821), an optical fiber (Thorlabs; M200L02S-UV), an optical switch (Ocean Optics; INLINE-TTLS), a custom bifuricated fiber optic reflection probe (Thorlabs; 6 fibers from the light source and 1 fiber to the spectrometer; the length from the light source to the cuvette or the spectrometer to the cuvette is 1 m each; the fiber used in this reflectance probe is a Thorlabs FG550UEC), a custom refurbished cuvette holder (Mark One Lifestyle Inc.), a quartz glass cuvette (Thorlabs; CV10Q3500F) with a custom aluminum mirrored surface, and a spectrometer (StellarNet; Silver Nova model, serial number 15040704). The spectrometer was placed in an environmental chamber (Espec BTL-433) at a temperature of 15 C and 70% relative humidity. The spectrometer responded to a wavelength range from 178 nm to 1115 nm with 1875 individual wavelengths. The data collection tool was the StellarNet software (SpectraWiz, version: 5.33), which stored the 128 scan data in “Episodic Scans” ep files. The computer running the tool was a dell laptop running Windows 8.

Data Collection

The data was collected according to AS-302: 1. Place a clean cuvette filled with distilled water in the cuvette holder 2. Take 128 scans of dark measurements at 20:20:200 ms 3. Take 128 scans of white measurements at 20:20:200 ms 4. Take 128 scans of dark and white measurements at 300:100:1000.

The tempertature compensation feature was **ON** for all measurements.

Data Analysis

The trials were collected as “episodic scans,” using SpectraWiz software, creating a file with an EP extension. These files were not readable in TextEditor or MS Office. Therefore, the files were read back in SpectrWiz as a 3D layout of 128 scans. Then each scan was saved as an SSM file (readable by Excel and TextEditor). A function was scripted in R programming language, to extract the data from all 128 SSM files into an R data.frame object.

Results

Dark Measurment

The dark measurements at different integration times 20,100,200,500, and 1000 ms, are shown in Figure 1. The temperature compensation feature centers the average of dark measruremts at zero counts. The dark measurement was independent of integration time, as shown in Figure 2. A total of 230,400 data points (i.e. 128 scans at 1800 wavelengths; wavelengths from 200 nm to 1100 nm, with increments of 0.5 nm) were used for each integration time. The dark signal was independent of the integration time.

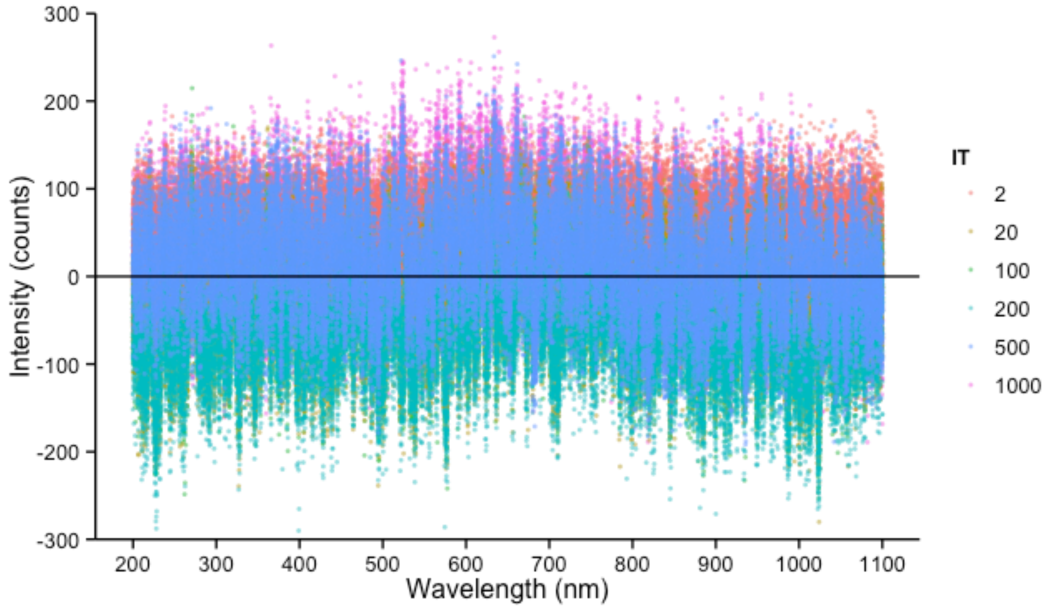

Figure 1. Dark measurement at different integration time.

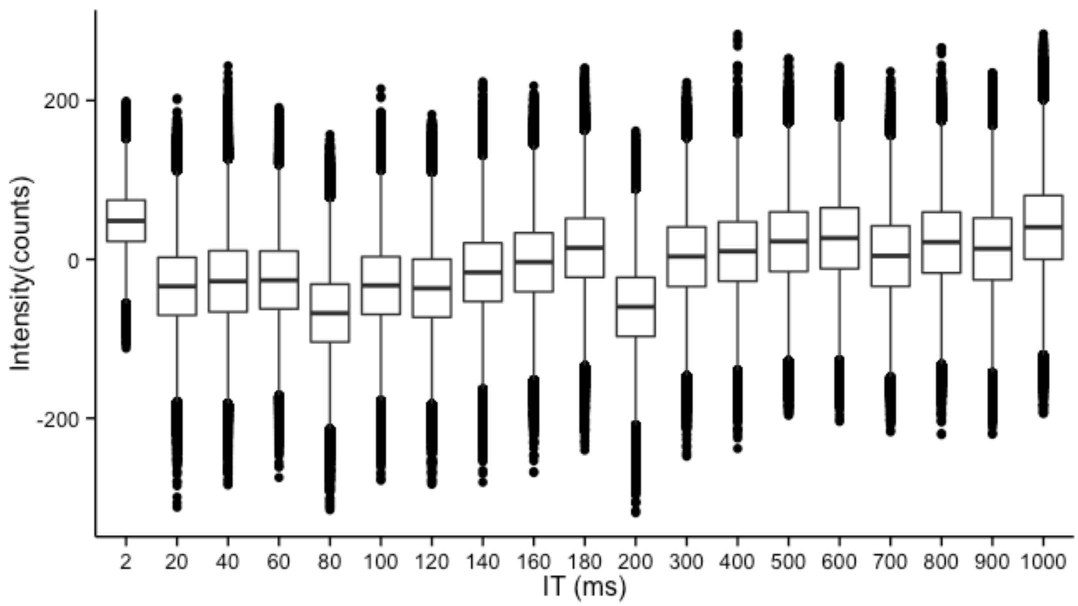

Figure 2. Boxplot of dark measurements at different integration time.

White Measurement

All the 128 scans (a trial) are graphed in Figure 2. The spectra response fairly increased linrearly by integration time. Each spectrum is a cloud of 128 scans (not the average signal at each wavelength). The signal response increased linearly by raising the IT (refer to **VA-85** for previous studies). A closer inspection of the spectrum at UV, VIS, and NIR regions demonstrated that the signal did not saturate in UV and NIR regions at ITs as high as 1000 ms. However, the maximum acheivable VIS signal, without clipping effect, happened at 200 ms integration time, as shown in Figures 3-5. As a conclusion, white signal increased linearly by increasing IT, while the dark signal was independent of IT. Therefore, one can conclude the signal-to-noise (SNR) value can be enhanced by increasing IT.

The spectrometer saturated at 58897 counts. According to Figures 3 and 4, the signal saturated around wavelength 490 nm and 932 nm. One can hypothesize that by paritioning the spectrum into 3 regions, each with an optimized IT value, the overall SNR value can be escalated. In the following sections, spectrometer SNR-value and noise-leve were studied in two settings: 1) **Non-partitioned:** spectroscopic response at 200 ms integration time all along the spectrum 2) **Partitioned:** spectroscopic response by partitioning (IT of 1000 ms in UV and NIR regions, and IT of 200 ms in VIS)

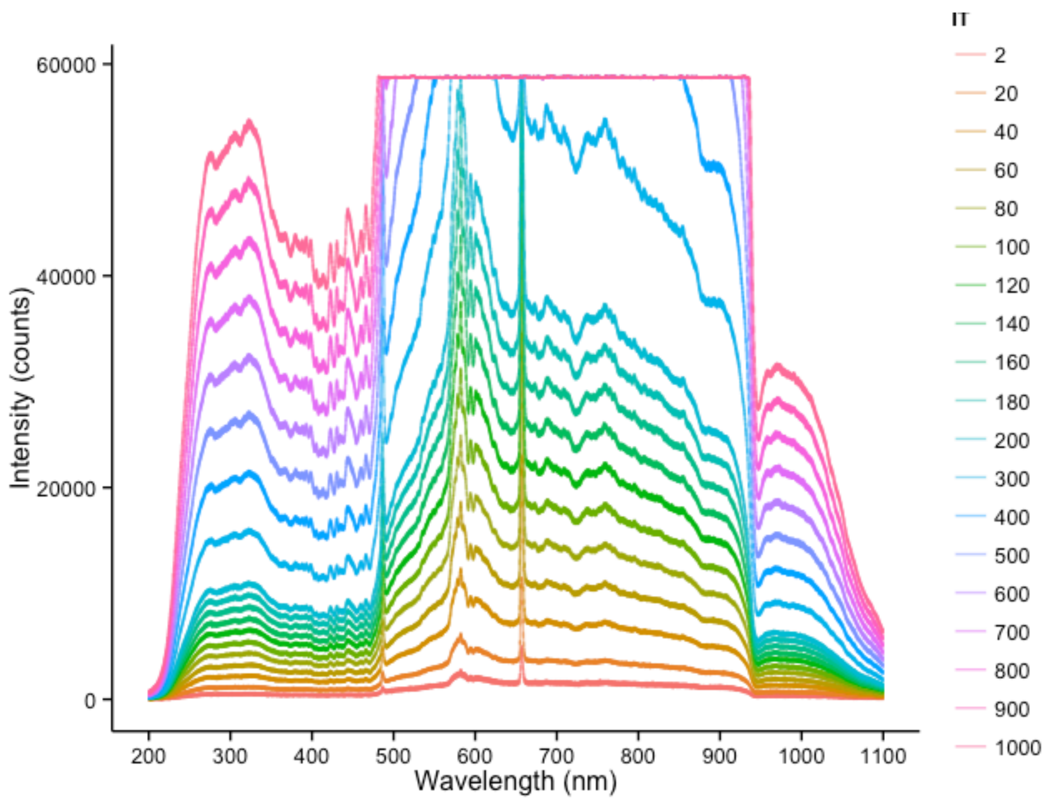

Figure 2. White trial at different integration time (IT).

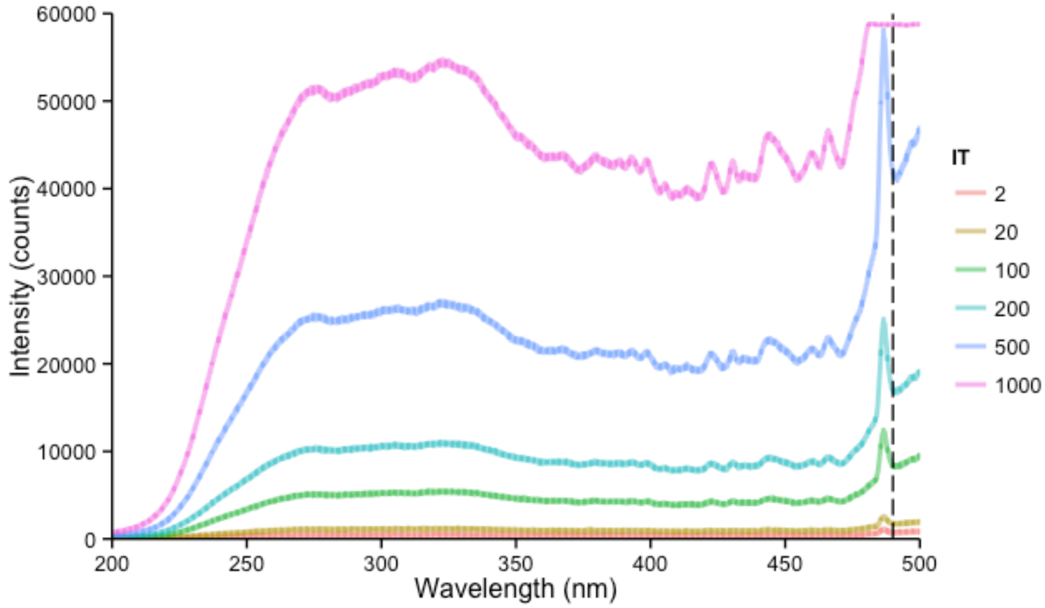

Figure 3. White trial in UV wavelength range, different integration time.

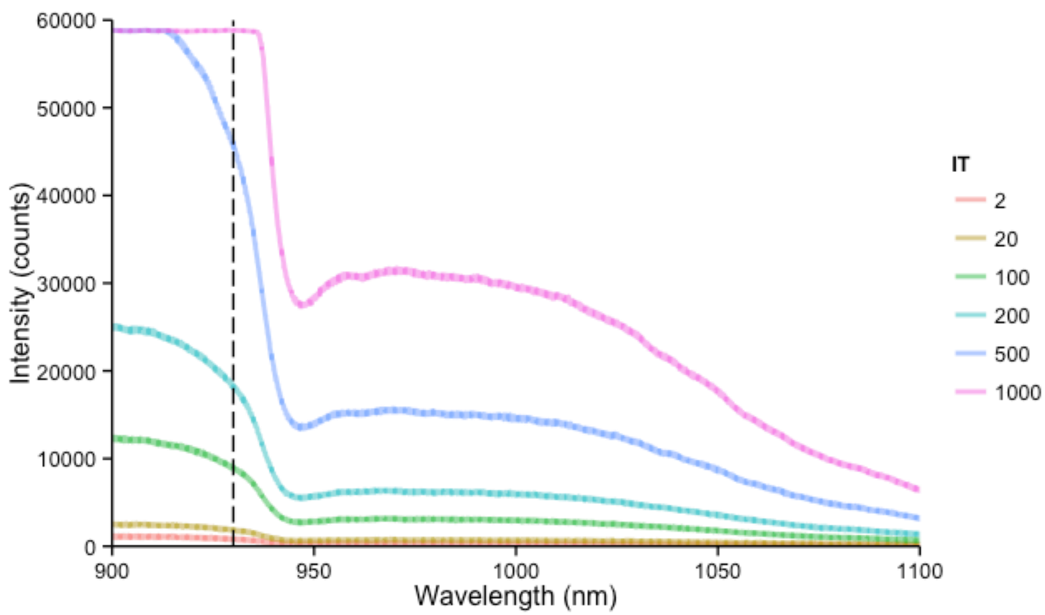

Figure 4. White trial in NIR wavelength range, different integration time.

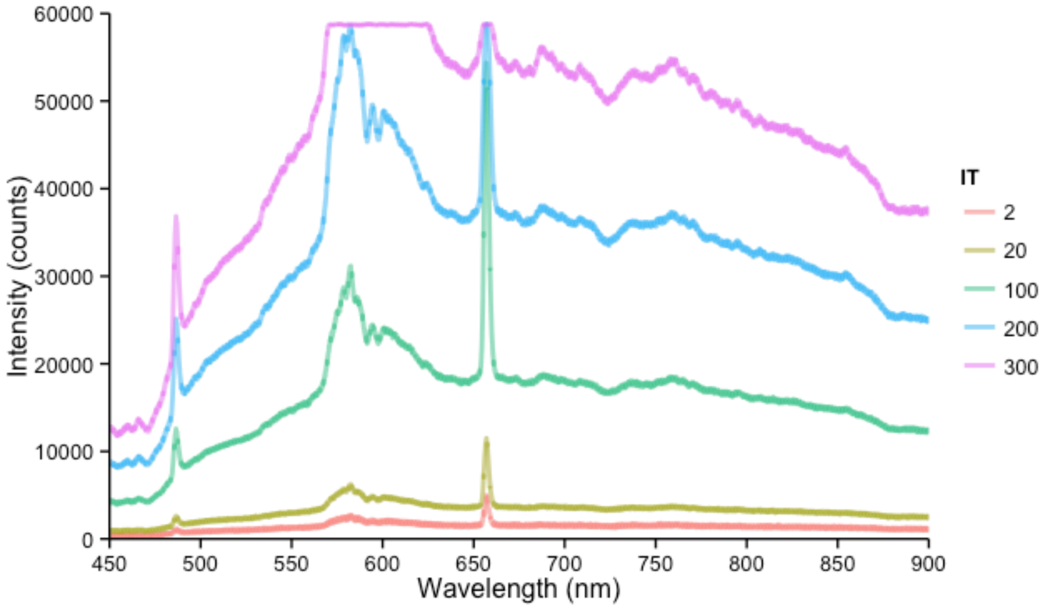

Figure 4. White trial in VIS wavelength range, different integration time.

Signal-to-Noise (SNR)

SNR value is defined as:

$$SNR^{IT}(\lambda) = \frac{\overline{W}^{IT}(\lambda) - \overline{D}^{IT}(\lambda)}{s^{IT}(\lambda)} \qquad Eq.1$$

Where $\overline{D}$ is the average dark signal, and $\overline{W}$ is the average white signal, and s is the standard deviation of white signal.

The SNR reponse of non-partitioned and partitioned spectra are shown respectively in Figures 5 and 6. The paritioned regions were graphed with differnt colors. For a better comparision, the partitioned and non-partitioned spectra are graphed together in Figure 7. The maxmim SNR values observed in non-partitioned spectrum were 150 in UV and 100 in NIR respectively. However, the maximum SNR values increased to 400 in UV and 300 in NIR, after partitioning. The **dark green** region was cause by overlapping VIS regions with IT at 200 ms.

The SNR response of spectrometer was also studied with respect to the difference of average white and average dark signal, as shown in Figure 8. The correlation can be modeled by $SNR^{IT}(\lambda) \propto \sqrt{\overline{W}^{IT}(\lambda) - \overline{D}^{IT}(\lambda)}$, which is in agreement with published by Ocean Optics.

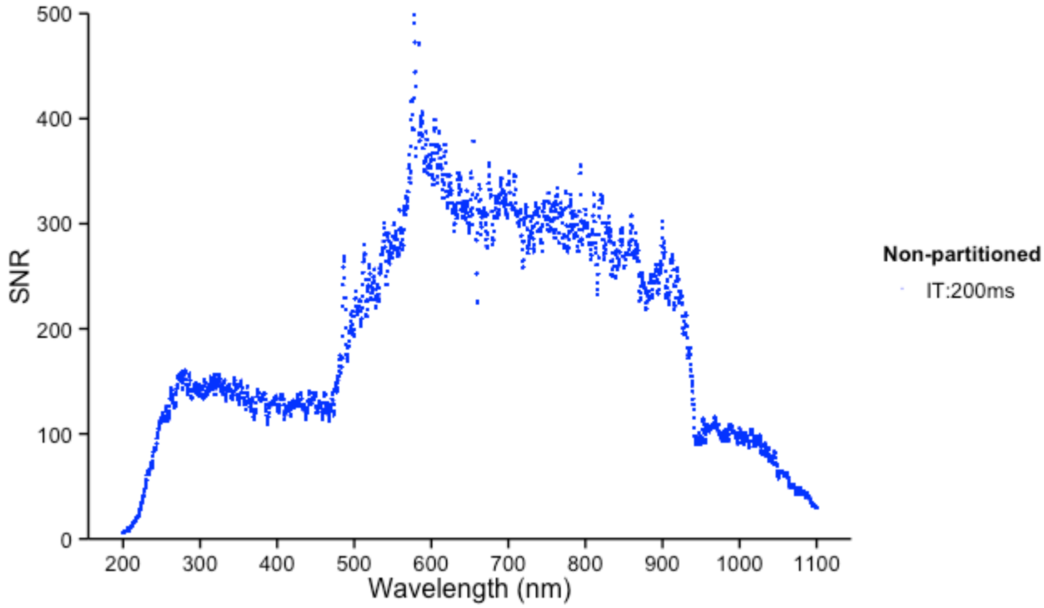

Fig 5. SNR reponse of non-partitioned spectrum at IT 200 ms.

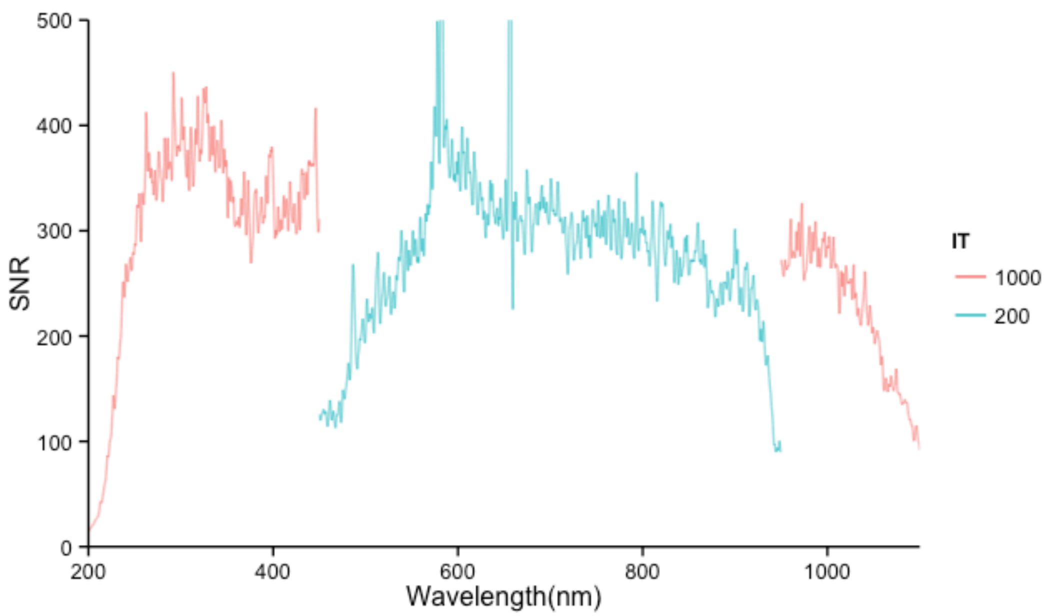

Figure 6. SNR reponse of partitioned spectrum. UV and NIR (red) at IT 1000 ms, VIS (green) at IT 200 ms.

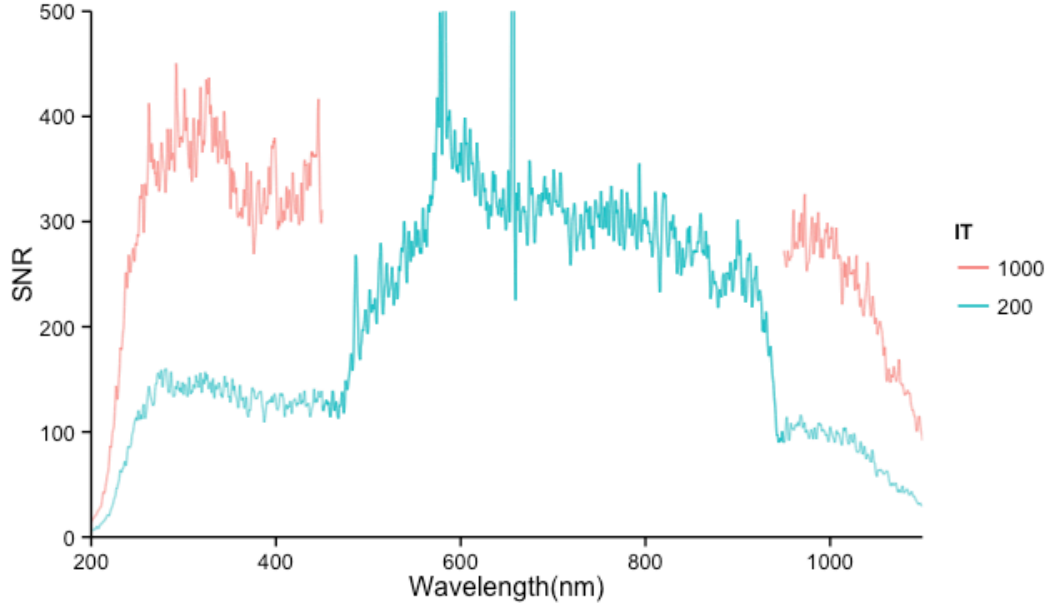

Figure 7. SNR comparision in between partitioned (red) and non-partitioned (green).

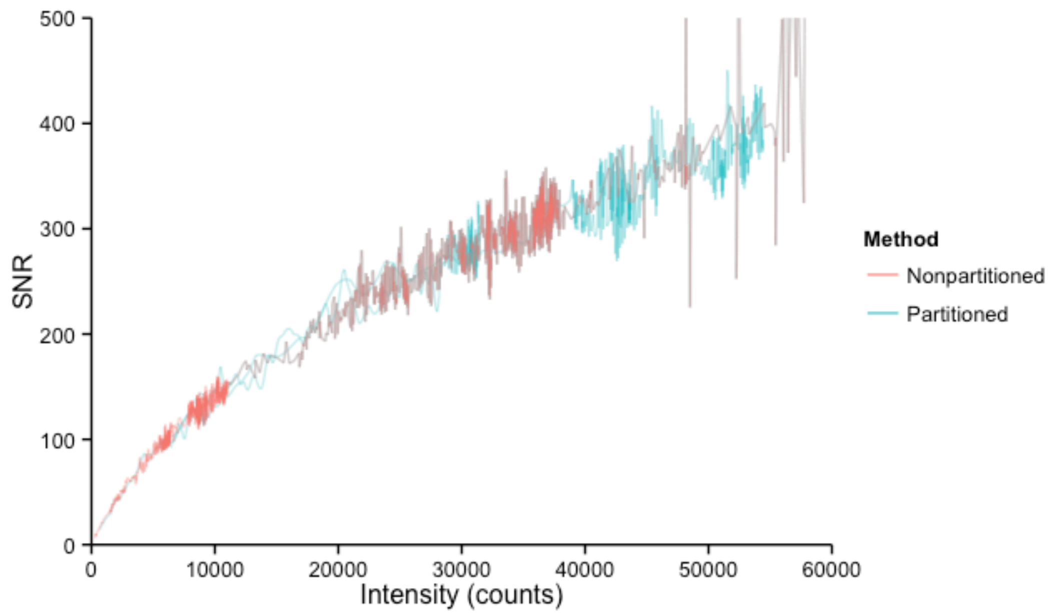

Figure 8. SNR reponse of partitioned (green) and non-partitioned (red) with respect to improvement in white signal.

Reflectance

Reflectance, a measure of individual white measurements normalized over average white signal, is defined in Equation 2:

$$R\ (\%) = \frac{W_i^{IT}(\lambda) - \overline{D}^{IT}(\lambda)}{\overline{W}^{IT}(\lambda) - \overline{D}^{IT}(\lambda)} \times 100 \qquad Eq.2$$

Where, W_i is individual white scans, $\overline{D}$ is the average dark signal, and $\overline{W}$ is the average white signal.

The results for reflectance calculation, for partitioned and non-partitioned spectra, can be seen in Figures 9 and 10. In non-partitioned case, an error margin of 10% for wavelengths below 250 nm, and a error margin of 5-10% for wavelength above 1050 nm were observed. In partitioned case, the error margin reduced to 2.5% for wavelengths below 250 nm, and reduced to less than 5% for wavelength above 1050 nm.

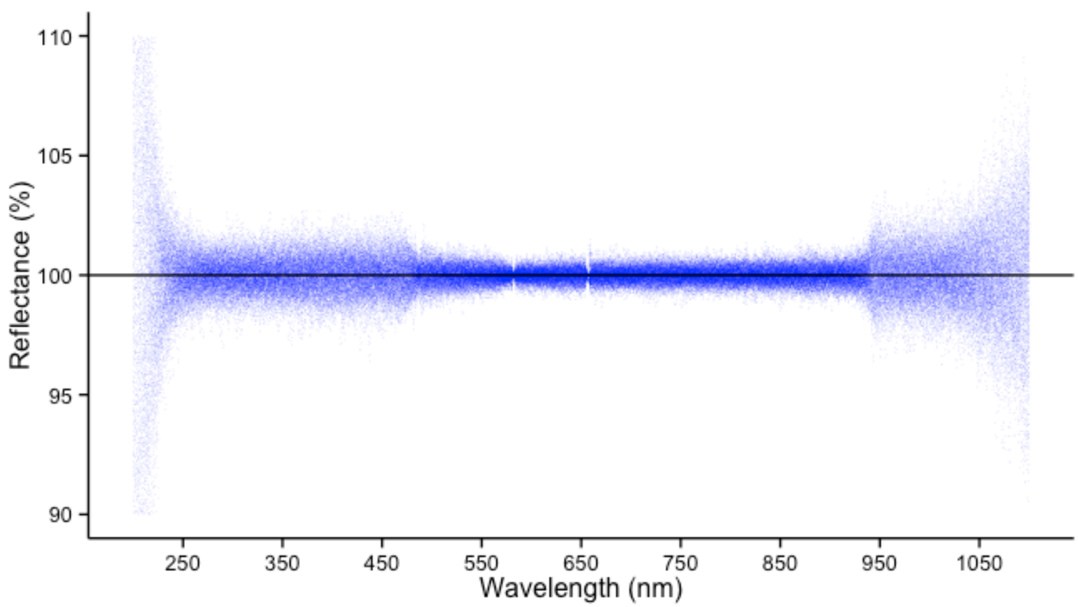

Figure 9. Reflectance response at 200 ms integration time.

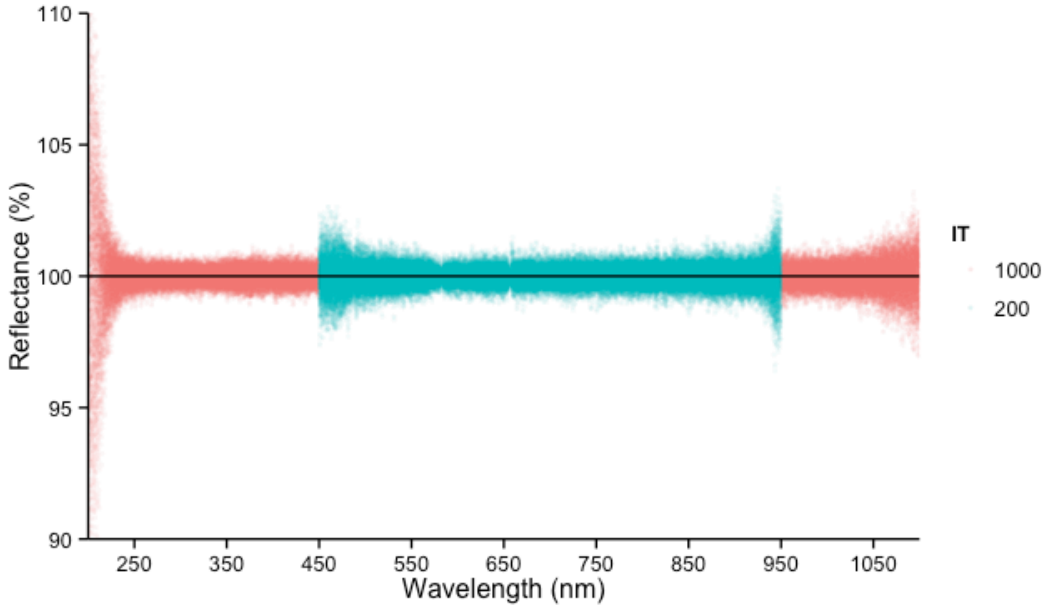

Figure 10. Reflectance response in partitioned specrtum.

Dark and White Noise

Dark noise, as the electronic noise, is defined as:

$$Dark\ Noise\ (\%) = \frac{R(\lambda)}{\overline{W}^{IT}(\lambda) - \overline{D}^{IT}(\lambda)} \times 100\ \ , R(\lambda) = Max\ D(\lambda) - Min\ D(\lambda) \quad Eq.3$$

Where R is the range of dark measurement at each wavelength, $\overline{D}$ is the average dark signal, and $\overline{W}$ is the average white signal.

White noise, as a statistical error, is defined as:

$$White\ Noise\ (\%) = \frac{R(\lambda)}{\overline{W}^{IT}(\lambda) - \overline{D}^{IT}(\lambda)} \times 100\ \ , R(\lambda) = Max\ W(\lambda) - Min\ W(\lambda)$$

$$Eq.4$$

Where R is the range of white measurement at each wavelength, $\overline{D}$ is the average dark signal, and $\overline{W}$ is the average white signal.

The dark and white noise were graphed for non-partitioned in partitioned situations in Figures 11 and 12. The red lines present the dark noise, while green ones present the white noise.

Emphasizing on non-partitioned spectrum, the dark noise was measured around 2.5% in UV range, reduced to less than 0.5% in VIS range, and increased to values as high as 10% at wavelengths above 1070 nm. The white noise was measured around 4-4.5% in UV range, reduced to 2-2.5% in VIS range, and increased to 7-10% in NIR range.

Focusing on partitioned spectrum, the dark noise was measured around 0.5%, and white noise was measured around 1.5-2% from wavelength 200-1050. Also, the spectrometer was able to distinguish between white and dark noise for wavelength above 1050-1100 nm.

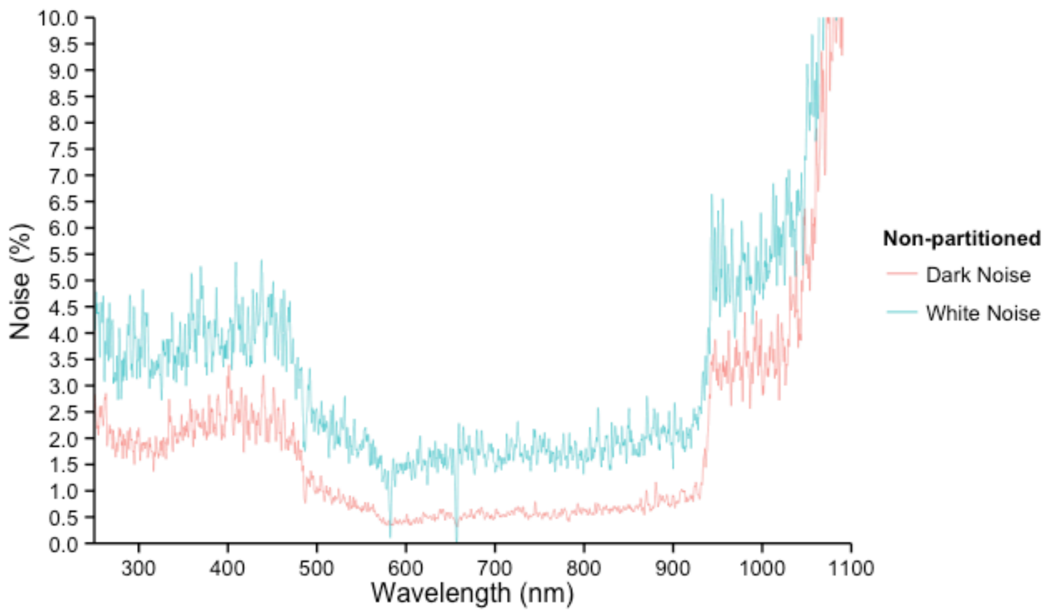

Figure 11. Calculated dark and white noise in non-partitioned spectrum.

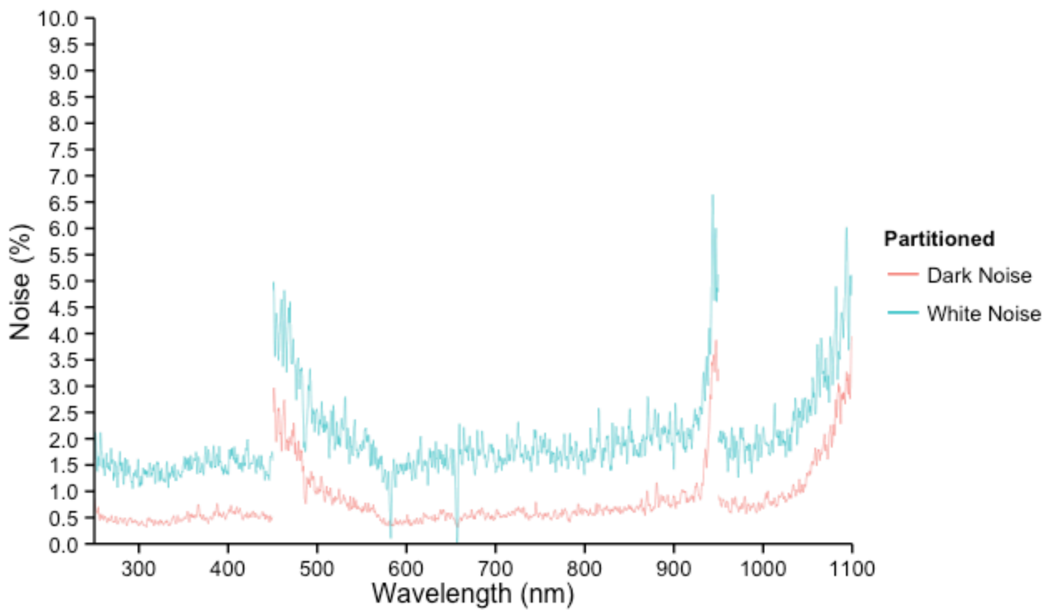

Figure 12.Calculated dark and white noise in partitioned spectrum.

One can also argue that dark and white noise can be defines as:

$$Dark\ Noise\ (\%) = \frac{3s(\lambda)}{\overline{W}^{IT}(\lambda) - \overline{D}^{IT}(\lambda)} \times 100 \qquad Eq.5$$

Where, 3s is three times standard deviation of dark signal at each wavelength.

White noise, as a statistical error, is defined as:

$$White\ Noise\ (\%) = \frac{3s(\lambda)}{\overline{W}^{IT}(\lambda) - \overline{D}^{IT}(\lambda)} \times 100 \qquad Eq.6$$

Where, 3s is three times standard deviation of white signal at each wavelength.

The dark and white noise were graphed for non-partitioned and partitioned situations in Figures 13 and 14. The red lines present the dark noise, while green ones present the white noise.

Emphasizing on non-partitioned spectrum, the dark noise was measured around 2.5% in UV range, reduced to less than 1% in VIS range, and increased to values as high as 10% at wavelengths above 1070 nm. The white noise was measured around

2-2.5% in UV range, reduced to 1-1.5% in VIS range, and increased to values greater than 5 % in NIR range.

Focusing on partitioned spectrum, the dark noise was measured maximum of 0.5%, and white noise was measured around 1% from wavelength 200-1050. Also, the spectrometer was able to distinguish between white and dark noise for wavelength above 1050-1100 nm.

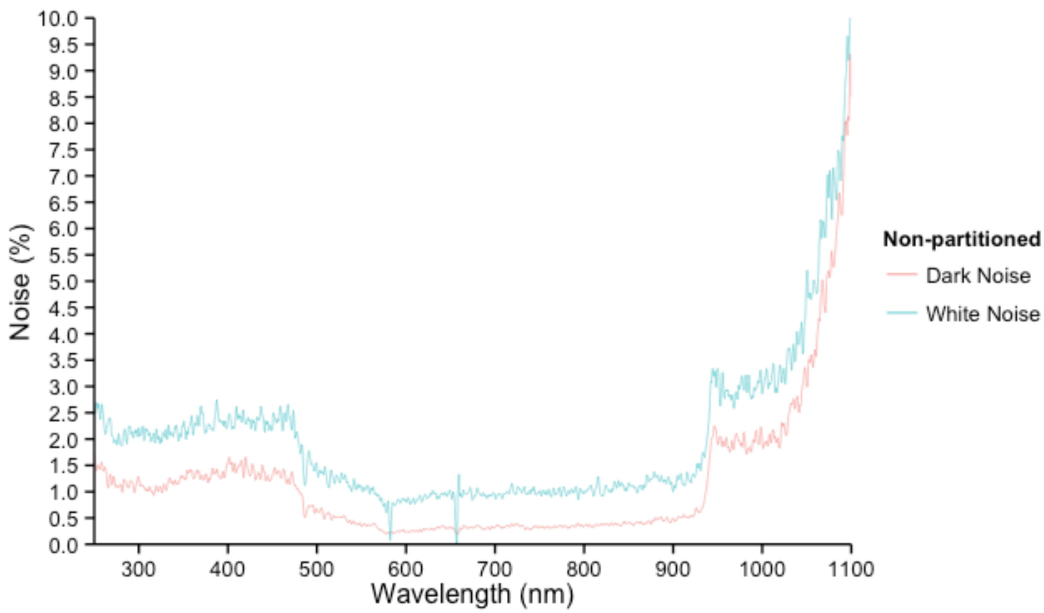

Figure 13. Calculated dark and white, using Equations 5 and 6, noise in non-partitioned spectrum.

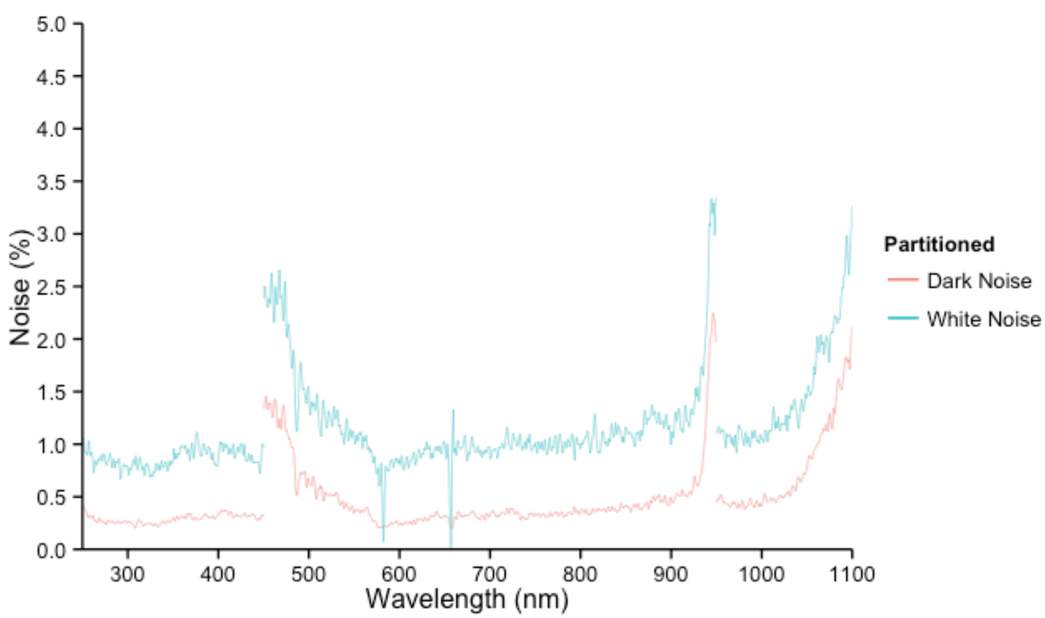

Figure 14. Calculated dark and white, using Equations 5 and 6 , noise in non-partitioned spectrum.

Conclusion

It was important to partition the spectrum into regions with optimum integration time, to increase the SNR values. It was noticed that VIS region saturated at IT values greater than 200 ms, while UV and NIR regions did not saturate at values as high as 1 second. Partitioning increased the SNR values and reduced dark/white noise level in UV and NIR regions. **The lowest calculated dark and white noise was measured to be 0.5% and 1% after partitioning.**