Environmental contributions and non-sample related impacts on the spectra from a handheld diffuse reflectance spectrometer

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BACKGROUND

Diffuse reflectance spectrometers (DRS) are becoming more portable and inexpensive, enabling handheld applied spectroscopy methods that are potentially useful to numerous fields. **However, future exploration of potential handheld DRS applications will require a detailed understanding of these sensors' capabilities and limitations.** Towards this end, we utilized **a 900 – 1700 nm handheld DRS (Innospectra NIR-S-G1 Reflective Spectrometer)** to examine three non-sample influences on spectra: sensor gain settings, sensor operation temperature, and environmental lighting conditions.

SENSOR GAIN EFFECTS

- **Methods:**
  - We scanned 2-99% Reflectance Standards with programmable gain amplifier (PGA) settings at powers of two from 1 to 64 and performed the USP <856> calibration procedure at each PGA.

FIGURE 1. Photometric Linearity per PGA

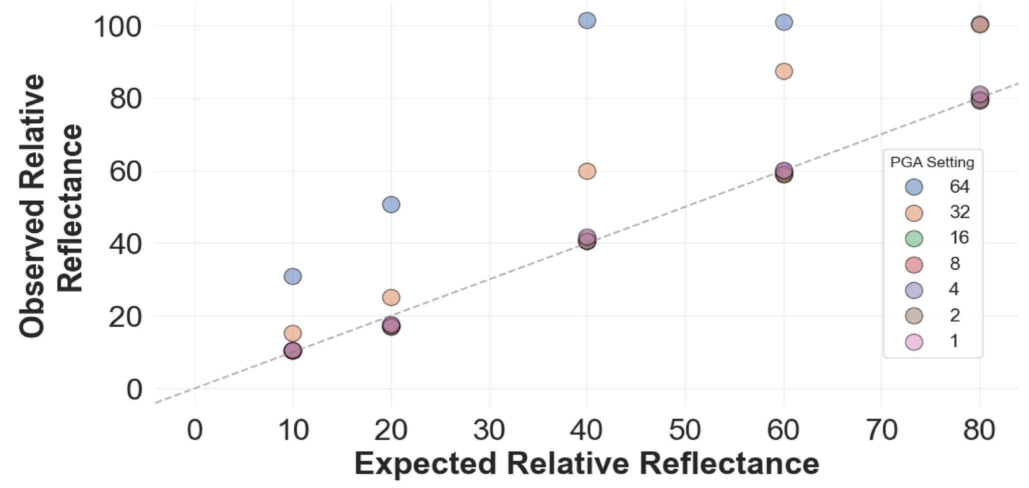


TABLE 1. USP <856> Calibration Results

PGA	Wavelength Verification	Photometric Linearity	Signal-to-Noise
64	Fail	Fail	Pass
32	Fail	Fail	Pass
16	Pass	Pass	Pass
8	Pass	Pass	Pass
4	Pass	Pass	Pass
2	Pass	Pass	Pass
1	Pass	Pass	Pass

- **Results:**
  - The sensor was able to comply with USP <856> for all PGAs 16 and below, while higher PGAs failed because they saturated the sensor.

OPERATING TEMPERATURE EFFECTS

- **Methods:**
  - We scanned a dysprosium, eridium, holmium, talc (DEHT) calibration puck every 30 seconds for an hour on 5 different sensors and tracked spectral changes alongside rising operation temperature. **Shaded areas below have R-Square values greater than 0.95**

FIGURE 2. DEHT Spectra Evolution with Temperature

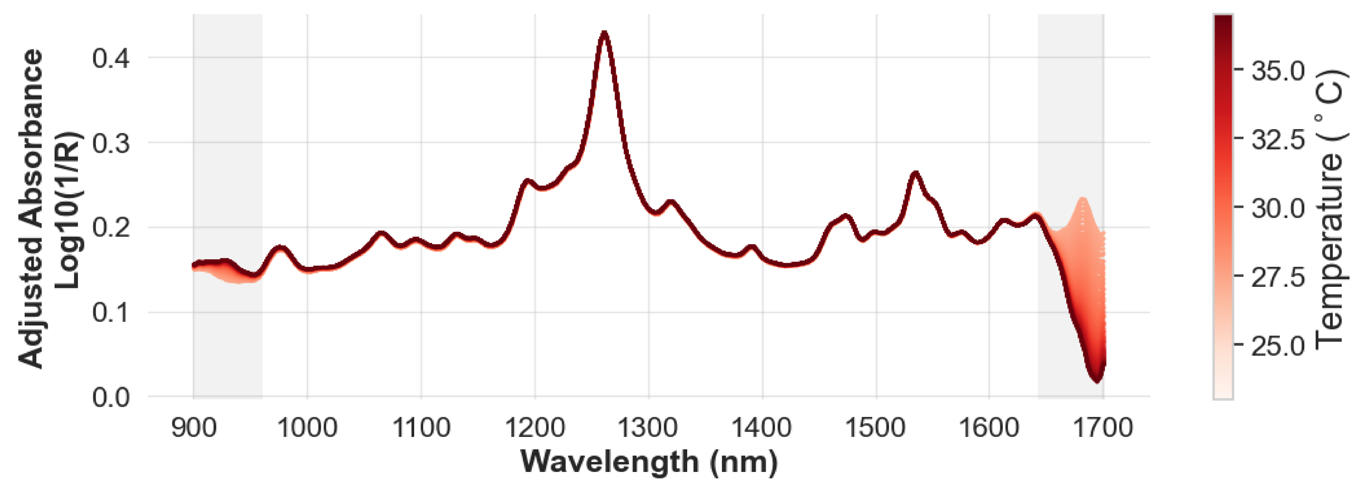
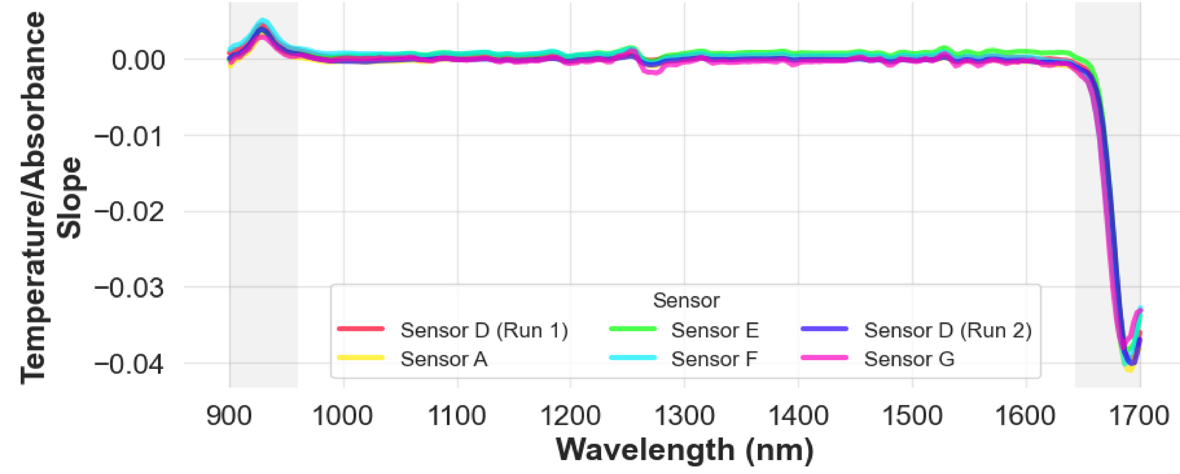


FIGURE 3. Temperature/Absorbance Slopes for 5 Sensors

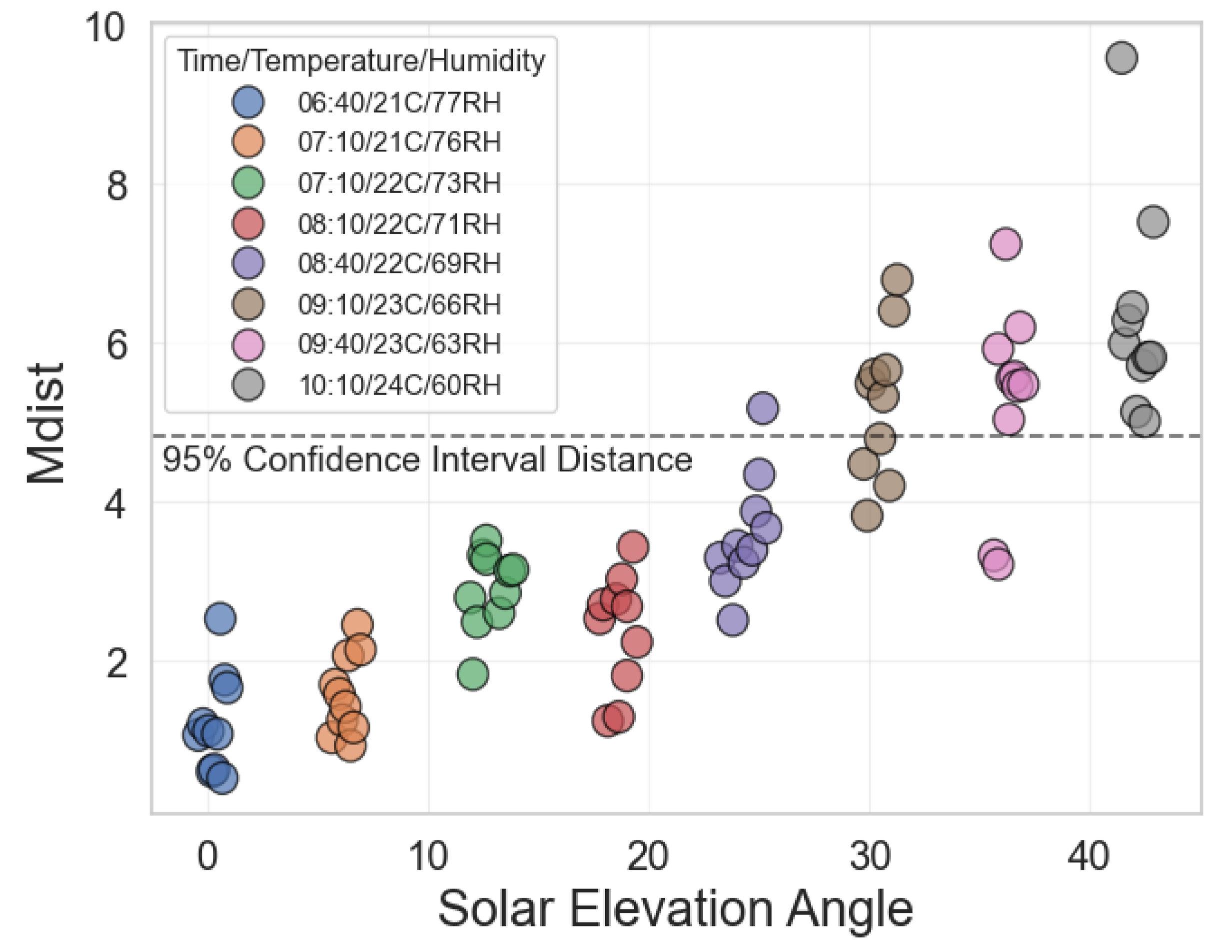


- **Results:**
  - The first and last 50 nm of 5 different sensors saw linear changes in absorbance associated versus operating temperature.

ENVIRONMENTAL SETTING EFFECTS

- **Methods:**
  - We scanned 10 clear HDPE vial caps outdoors every 30 minutes from 6:40 AM to 10:10 AM and tracked the changes in the Mahalanobis distances of their principal components relative to 30 different clear HDPE vial caps scanned under controlled laboratory conditions.

FIGURE 4. Solar Angle Effect on HDPE Mahalanobis Distances



- **Results:**
  - We observed that Mahalanobis distances for the vial caps increased with the solar elevation angle, eventually surpassing the 95% confidence interval threshold distance.

CONCLUSIONS AND RECOMMENDATIONS

We found (a) that handheld DRS could pass USP <856> calibration if the gain was set not to saturate the DRS, (b) the precise DRS wavelength ranges that experience changes with operating temperature and that these regions have linear temperature/absorbance relationships, and (c) that the solar elevation angle has a significant effect on spectra collected outdoors. We recommend utilizing PGAs 16 and below, truncating spectra by 50 nm at both ends, and shaping all statistical models around the intended environmental setting. These results better enable field usage of handheld NIR spectrometers by examining key sources of error and laying the groundwork for potential fixes.

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