The Third Global Workshop on Proximal Soil Sensing (Potsdam, Germany)

Analysis of the Repeatability of Soil Spectral Data Obtained Using Different Measurement Techniques

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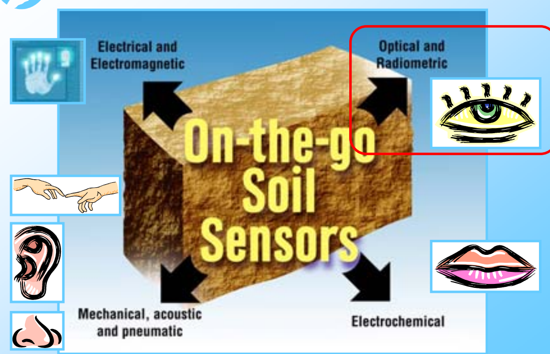
McGill



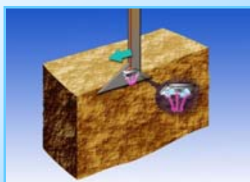
Optical Sensors

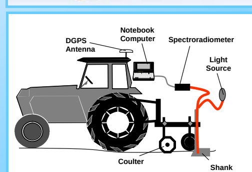
Subsurface Soil Reflectance Sensors

- Visual
- Near-infrared
- Mid-infrared

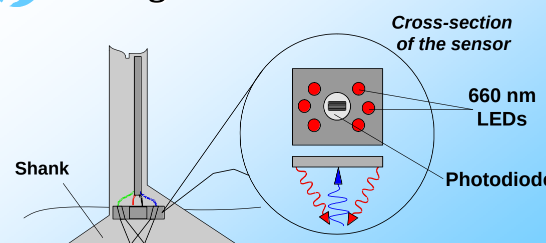
- Image analysis
- Polarized light

- *Organic matter (carbon) content*
- *Soil texture*
- *Cation exchange capacity (CEC)*
- *Soil water content*
- *Soil pH*
- *Mineral nitrogen and phosphorous*



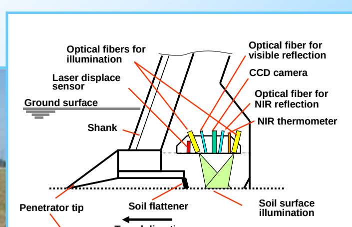


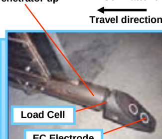
Organic Matter Sensor



Purdue University (West Lafayette, Indiana)

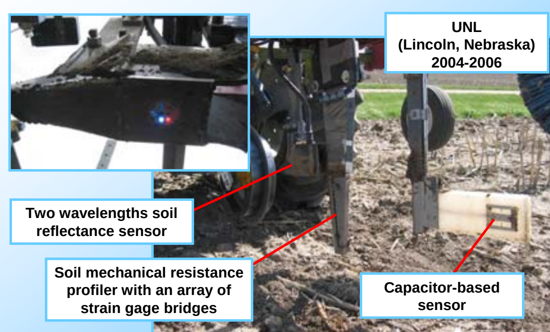
Traveling Spectrophotometer



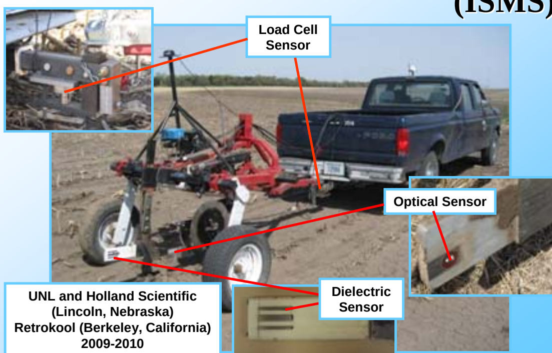


Tokyo University of Agriculture and Technology (Tokyo, Japan)

Integrated Soil Physical Properties Mapping System (ISPPMS)



Integrate Soil Mapping System (ISMS)

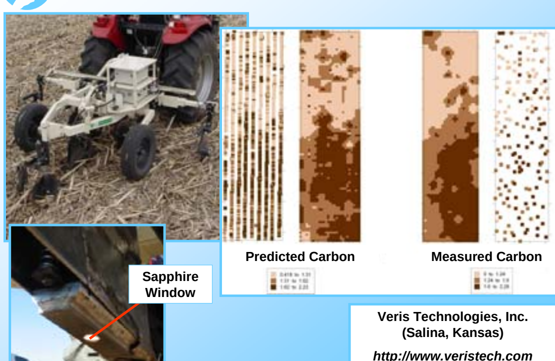


Veris® OpticMapper™

Veris Technologies, Inc. (Salina, Kansas)
http://www.veristech.com

660 and 940 nm

VIS/NIR Spectrophotometer



Veris Technologies, Inc. (Salina, Kansas)
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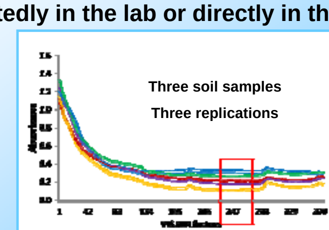
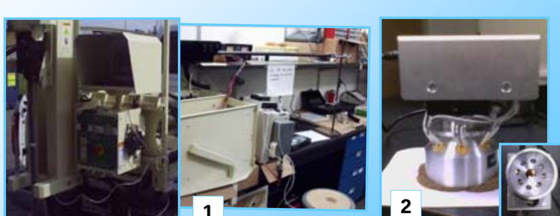
Objective

Assess the repeatability of unprocessed visible, near-infrared, and mid-infrared spectra as well as their most common derivatives when the same soil samples were measured repeatedly in the lab or directly in the field



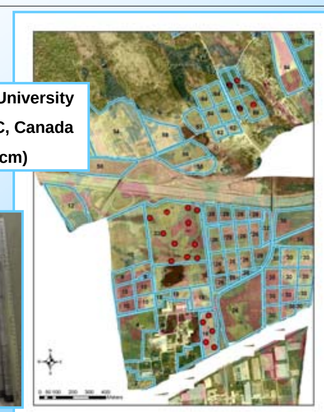
Instruments

1. Visible/Near-Infrared spectroscopy (Vis-NIR) - 400-1000 nm and 1100-2200 nm
2. Diffuse Reflectance Variable Filter Array Mid-Infrared spectroscopy (MIR) - 2780-5096 nm

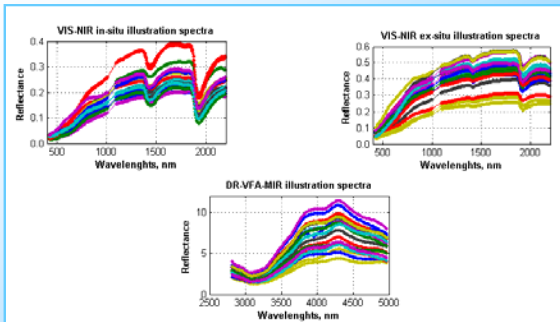


Sites

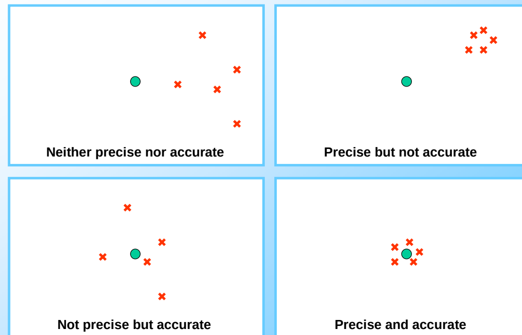
Macdonald Farm, McGill University
Ste-Anne-de-Bellevue, QC, Canada
20 samples (top 15 cm)



Spectra Examples



Precision versus Accuracy



Relative Error Definition

Standard error
Root mean squared error (RMSE)

Data spread
Standard deviation (SD_{SA})

Ratio of Prediction over Deviation (RPD)
Ratio of Spread over Error (RSE)

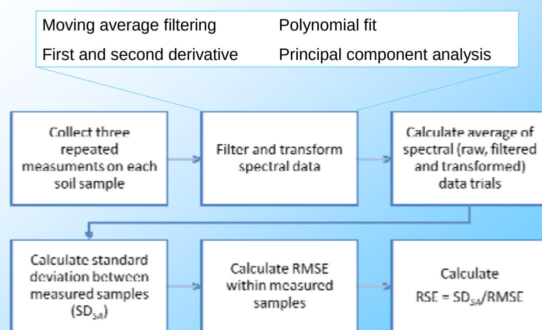
	SS	DF	MS	F-stat	p-value	F-crit
Soils	1.1817	19	0.0622	21.7601	2.17681E-15	1.8529
Error	0.1143	40	0.0029			
Total	1.2960	59				

20 soil samples with 3 replicated measurements

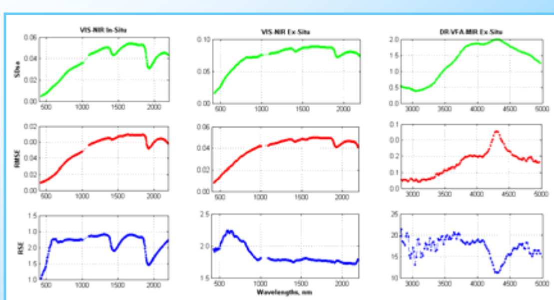
$$RSE = \frac{SD_{SA}}{RMSE} = \sqrt{\tfrac{1}{3} F_{stat}}$$

RSE > 0.79

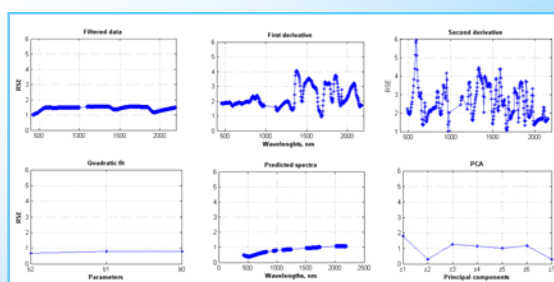
Methodology



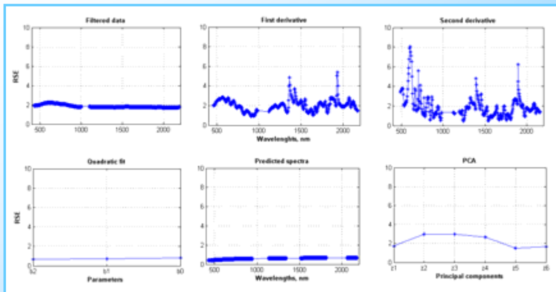
Raw Spectra Analysis



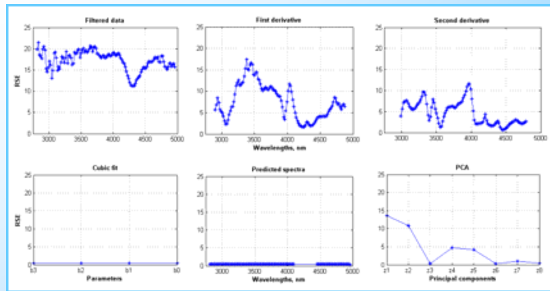
Vis-NIR (in-situ)



Vis-NIR (ex-situ)



MIR (ex-situ)



RSE Summary

Equipment and Method	Data Transformation	RSE				
		Min	25%	Median	75%	Max
VIS NIR *In-situ*	Filtered	1.01	1.39	1.49	1.54	1.56
	Polynomial fit	0.40	0.64	0.86	1.00	1.08
	First derivative	0.92	1.84	2.00	2.90	4.05
	Second derivative	1.04	1.83	2.36	3.19	5.93
	Principal components	0.29	0.48	1.15	1.24	1.80
VIS NIR *Ex-situ*	Filtered	1.72	1.76	1.78	1.85	2.24
	Polynomial fit	0.42	0.56	0.63	0.66	0.67
	First derivative	0.92	1.63	2.03	2.40	5.38
	Second derivative	0.47	1.20	1.68	2.25	8.07
	Principal components	1.52	1.64	2.21	2.98	3.00
MIR *Ex-situ*	Filtered	11.28	15.73	17.84	18.82	21.41
	Polynomial fit	0.40	0.44	0.47	0.47	0.48
	First derivative	1.64	4.11	6.88	10.78	17.40
	Second derivative	0.68	2.23	4.18	6.82	11.58
	Principal components	0.33	0.39	2.61	7.83	13.67

Summary

- **The filtered MIR measurements had the highest relative reproducibility across the entire spectrum**
- **RSEs for the derivatives were dependent on the wavelength**
- **Vis-NIR data ex-situ measurements were more reproducible than those conducted in natural soil conditions within a 0.5 m distance from each other**
- **For both in-situ and ex-situ Vis-NIR data, the second derivative (spectral inflection data) yielded data that had the highest relative reproducibility in certain parts of the spectrum**
- **Other types of data transformation did not yield higher RSE estimates**

Next Steps

- **Six different instruments**
- **Five different datasets**
- **Precision versus accuracy analysis**
- **Optimized system for in-situ operation**

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