



## Introduction & Aims

Diffuse reflectance spectroscopy (DRS) is attracting much interest in the soil science community. It has a number of advantages over conventional methods of soil analyses: DRS is rapid, timely, cheaper and hence more efficient at obtaining the data when a large number of samples and analysis are required. Moreover, a single spectrum may be used to assess various physical, chemical and biological soil properties.

Until now, research in soil spectroscopy has focused on spectral calibration and prediction of soil properties using multivariate statistics. In this instance we show how these predictions may be used in an inference system to predict other important and functional soil properties using pedotransfer functions (PTFs).

Our aims are:

- (i) to use of soil spectral calibration and predictions as input and complement to a soil inference system (SPEC-SINFERS),
- (ii) to demonstrate the implementation of SPEC-SINFERS

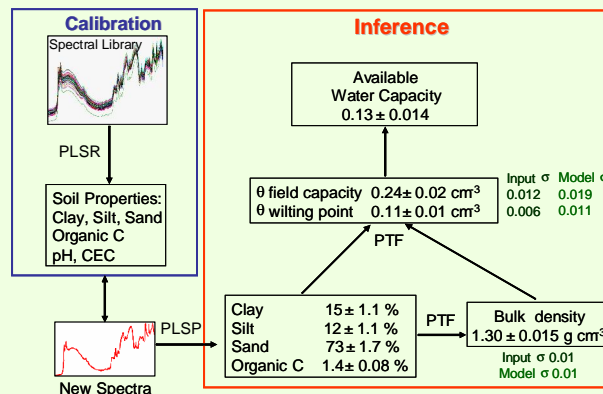
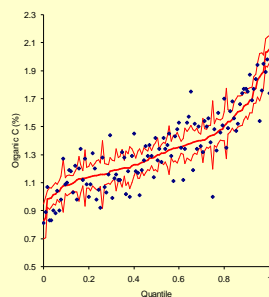
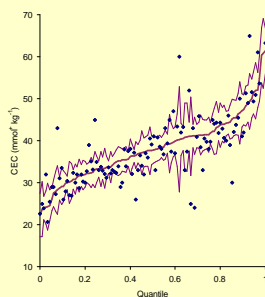
## Materials & Methods

Soil data

- Sampled 116 A-horizon (0-20 cm) soil samples. These were oven dried and ground (< 2mm)
- Soil analyses: pH, Organic C, Sand, Silt, Clay, CEC
- Soil samples scanned using a FT-MIR spectrometer.
- The actual spectral range used in the analysis was 2500 – 19936 nm (4000 - 502 cm<sup>-1</sup>). Reflectance transformed to Log<sub>10</sub>(1/R)
- Partial Least Squares Regression (PLSR) was used to construct predictive models.
- Both model and input uncertainties were quantified:
  - Model uncertainty : Bootstrap
  - Input uncertainty : LHS with Monte Carlo Simulation
- Model and input uncertainties were propagated through the calculations

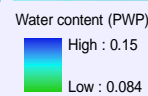
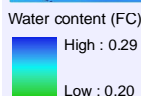
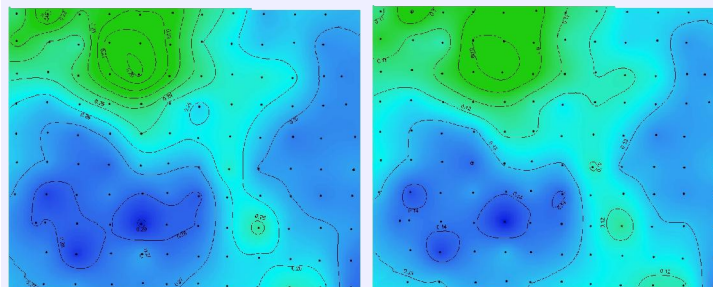
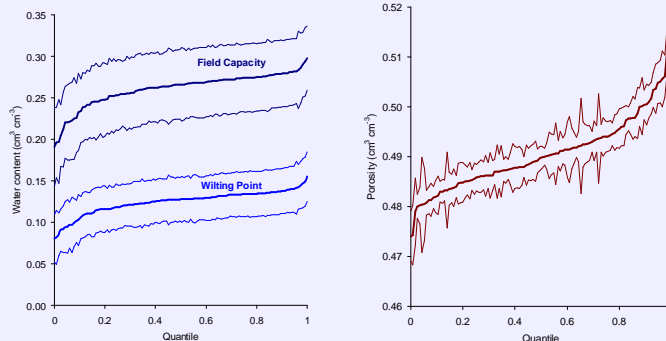
## Results

Variables	Model	Input	R <sup>2</sup>	RMSE
Clay content dag kg <sup>-1</sup>	PLSR	MIR Spectra	0.79	1.39
Sand content dag kg <sup>-1</sup>	PLSR	MIR Spectra	0.82	2.16
pH in H <sub>2</sub> O pH unit	PLSR	MIR Spectra	0.86	0.092
pH in CaCl <sub>2</sub> pH unit	PLSR	MIR Spectra	0.92	0.068
Organic C dag kg <sup>-1</sup>	PLSR	MIR Spectra	0.77	0.13
Cation exchange capacity mmol(+) kg <sup>-1</sup>	PLSR	MIR Spectra	0.69	5.36
Mineral bulk density g cm <sup>-3</sup>	Neural Network	Clay, Silt, Sand, Bulk Density	0.52	0.152
Particle density g cm <sup>-3</sup>	Linear Regression	Organic C	0.98	0.055
Lower plastic limit g g <sup>-1</sup>	Linear Regression	Clay, Organic matter	0.54	
Upper plastic limit g g <sup>-1</sup>	Linear Regression	Clay, Organic matter	0.66	
Soil mechanical resistance kPa	Linear Regression	Clay, Sand, Organic C, Bulk density	0.83	585.6
Water retention: Field capacity (-10 kPa) cm <sup>3</sup> cm <sup>-3</sup>	Neural Network	Clay, Silt, Sand, Bulk Density, Organic C	0.64	0.057
Willing Point (-1500 kPa) cm <sup>3</sup> cm <sup>-3</sup>	Neural Network	Clay, Silt, Sand, Bulk Density, Organic C	0.66	0.050
Saturated hydraulic conductivity log (mm h <sup>-1</sup> )	Neural Network	Clay, Silt, Sand, Bulk Density, $\theta$ at -10 kPa	0.60	1.50
pH Buffering Capacity mmol H <sup>+</sup> kg <sup>-1</sup> pH <sup>-1</sup>	Linear Regression	Clay, Silt, Sand, Organic Carbon	0.79	



Spectral calibration (left box) and example of a soil inference system (right box). PLSR model to predict soil properties (e.g. clay, silt, sand, and OC) along with their uncertainties. These are inputted into the inference system to calculate other properties (e.g. bulk density). The resulting input and model uncertainties are quantified. These are then used to calculate  $\theta_{FC}$  and  $\theta_{WP}$  and AWC. Uncertainties are propagated.

We show results for: soil water holding capacity



## Conclusions

- Diffuse spectroscopy provides rapid measurement of soil properties, Although the accuracy of the basic soil properties obtained from spectroscopy is lower than laboratory analysis, the efficiency of the measurements in terms of cost and time is much higher
- SPEC-SINFERS uses soil spectra to estimate various basic soil properties which are then to infer other important and functional soil properties via pedotransfer functions. The important feature of SPEC-SINFERS is the propagation of both input and model uncertainties.

## References

- McBratney, A.B., Minasny, B., Cattle, S.R., Vervoort, R.W., 2002. From pedotransfer functions to soil inference systems. *Geoderma* 109, 41-73.
- Viscarrá Rosell, R.A., Walvoort, D.J.J., McBratney, A.B., Janik L.J. and Skjemstad, J.O. 2005. Visible, near-infrared, mid-infrared or combined diffuse reflectance spectroscopy for simultaneous assessment of various soil properties. *Geoderma* (available on-line)