Imaging Spectroscopy for Soil Applications

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Image Spectroscopy – Some Milestones


1984-AVIRIS
1987-GER
1992-CASI
1994- AISA
1994-MIVIS
1996- HYMAP
1997- DAIS
1999, 2000 - MODIS, ASTER
2000-HYPERION
2001-CHRIS-PROBA
2003-AISA-ES
2006- AVIRIS*
2007-ARES
2010-EnMAP
IS in Science (2)

% from the total published papers

<table>
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<th>Year</th>
<th>1995</th>
<th>2000</th>
<th>2005</th>
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<td>5.14%</td>
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IGARSS and 27th Canadian Symposium on Remote Sensing, Denver, Colorado August 2, 2006: State of Science of Environmental Application of Imaging Spectroscopy in honor of Prof. A. Goetz
**IS in IGARSS**

**Image Spectroscopy Sessions**
- 1990, Maryland US – 0/80 = 0%
- 2006, Denver US – 7/80 = 9%

(not including other sessions with IS oriented issues)

**RADAR & SAR sessions**
- 1990, Mariland US -15/120 = 12.5%
- 2006, Denver US – 21/120 = 17.5%

First met with Alex

Honor to Alex

IGARSS and 27th Canadian Symposium on Remote Sensing, Denver, Colorado August 2, 2006: State of Science of Environmental Application of Imaging Spectroscopy in honor of Prof. A. Goetz
Soil: "The upper layer of the earth which may be dug, plowed, specifically, the loose surface material of the earth in which plants grow." (Thompson 1957)

Soil is composed of:
- Clay
- Silt
- Sand
- Organic matter
- Carbonates
- Iron oxides
- Water
- Particle size
- Air

Return Impact
IS: The acquisition of images in hundreds of registered, contiguous spectral bands such that for each picture element it is possible to complete reflectance spectrum (Goetz 1994)
Soil Spectroscopy


5 spectral types in USA

Main Soil Chromophores

Ben-Dor E., and A. Banin 1995b, Near infrared analysis (NIRA) as a Simultaneously method to evaluate spectral featureless constituents in soils., Soil Science 159:259-269

Figure 2

Soil Chromophores

Spectral Assignments for Soil Constituents

Vibration

Charge Transfer

Crystal Field

Intensity

- Strong
- Weak
- Very Weak

WAVELENGTH (μm)

0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1

Soil Chromophores in honor of Prof. A. Goetz

IGARSS and 27th Canadian Symposium on Remote Sensing, Denver, Colorado August 2, 2006: State of Science of Environmental Application of Imaging Spectroscopy in honor of Prof. A. Goetz
Quantitative Method for spectral based matter properties (1)

Principal components methodology
- Matter properties expressed as a linear function of its reflectance spectral data:

\[ y_{30X1} = 1_{30X1} b_0 + C_{30X119} b_{119X1} + e_{30X1} \]

Cheng-Wen et al. (2001)
Quantitative Method for spectral based material properties (2)

Quantitative Method for spectral based SOIL properties

NIRS


NIRS is a chemometrics method where NIR-SWIR spectral region is used to predict chemical constituents of a given matter.
Soil- NIRS summary


<table>
<thead>
<tr>
<th>Soil attribute</th>
<th>Spectral region</th>
<th>Spectral range (nm)</th>
<th>Multivariate methoda</th>
<th>( n_{\text{calib}} )</th>
<th>( n_{\text{valid}} )</th>
<th>RMSE</th>
<th>( R^2 )</th>
<th>Authors</th>
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<td>$R^2$</td>
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<td></td>
<td>Islam et al. (2003)</td>
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<td>NIR</td>
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<td>PLSR (17)</td>
<td>177</td>
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<td>0.80</td>
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<td>OC; g/kg</td>
<td>VIS–NIR</td>
<td>400–2498</td>
<td>PLSR (6)</td>
<td>76</td>
<td>32</td>
<td>0.62</td>
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</tr>
<tr>
<td>OC; dag/kg</td>
<td>VIS–NIR</td>
<td>350–1050</td>
<td>PLSR (5)</td>
<td>43</td>
<td>25</td>
<td>0.36</td>
<td></td>
<td>Viscarra Rossel et al. (2003)</td>
</tr>
<tr>
<td>OC; %</td>
<td>UV–VIS–NIR</td>
<td>250–2500</td>
<td>PCR</td>
<td>121</td>
<td>40</td>
<td>0.76</td>
<td></td>
<td>Islam et al. (2003)</td>
</tr>
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<td>OM; %</td>
<td>MIR</td>
<td>2500–25,000</td>
<td>PLSR (4)</td>
<td>31 x-val</td>
<td>0.72</td>
<td>0.98</td>
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<td></td>
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<tr>
<td>OM; %</td>
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<td>39</td>
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</tr>
<tr>
<td>OM; %</td>
<td>NIR</td>
<td>400–1100</td>
<td>NN</td>
<td>41</td>
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<td>Daniel et al. (2003)</td>
<td></td>
</tr>
<tr>
<td>OM; %</td>
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<td>400–2400</td>
<td>SMLR (606, 1311, 1238)</td>
<td>15</td>
<td>10</td>
<td>0.65</td>
<td></td>
<td>Shibusawa et al. (2001)</td>
</tr>
</tbody>
</table>

P (avail.); mg/kg               | MIR             | 2500–25,000       | PLSR                | 186                                          | 0.07  |       | Janik et al. (1998)         |
<p>| P (avail.); mg/kg              | VIS–NIR         | 400–1100          | NN                  | 41                                          | 0.81  |       | Daniel et al. (2003)        |
| pH                             | MIR             | 2500–20,000       | PLSR                | 180 x-val                                   | 0.72  |       | Janik and Skjemstad (1995)  |
| pH                             | NIR             | 1100–2300         | PLSR (8)            | 120|59                                        | 0.74  |       | Reeves and McCarty (2001)   |
| pH                             | NIR             | 1100–2498         | PLSR (11)           | 120|59                                        | 0.73  |       | Reeves et al. (1999)        |
| pH                             | VIS–NIR         | 350–2500          | MARS                | 505|253                                        | 0.43  | 0.70  | Shepherd and Walsh (2002)   |
| pH                             | MIR             | 2500–25,000       | PLSR                | 183                                          | 0.67  |       | Janik et al. (1998)         |</p>
<table>
<thead>
<tr>
<th>Soil attribute</th>
<th>Spectral region</th>
<th>Spectral range (nm)</th>
<th>Multivariate method&lt;sup&gt;a&lt;/sup&gt;</th>
<th>$n_{\text{calib}}$</th>
<th>$n_{\text{valid}}$</th>
<th>RMSE</th>
<th>$R^2$</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>OC; %</td>
<td>MIR</td>
<td>2500–25,000</td>
<td>PLSR</td>
<td>188</td>
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<td>0.93</td>
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<td>OC; (acidified soil) g/kg</td>
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<td>0.97</td>
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<tr>
<td>OC; %</td>
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<td>MLR (1744, 1870, 2052)</td>
<td>72</td>
<td>48</td>
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<td>Dalal and Henry (1986)</td>
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<tr>
<td>OC; %</td>
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<td>RBFN</td>
<td>140</td>
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<td>OC; g/kg</td>
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<td>0.07</td>
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<td>PLSR (11)</td>
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<td>59</td>
<td>0.73</td>
<td></td>
<td>Reeves et al. (1999)</td>
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<tr>
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<td>350–2500</td>
<td>MARS</td>
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<tr>
<td>pH&lt;sub&gt;Ca&lt;/sub&gt;</td>
<td>MIR</td>
<td>2500–25,000</td>
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<td>183</td>
<td></td>
<td>0.67</td>
<td></td>
<td>Janik et al. (1998)</td>
</tr>
</tbody>
</table>
Conclusions

• Soil Spectra consists of many interesting chromophores
• Quantitative analysis of soil spectra is possible (NIRS)
• Soil is a complex system
Idea: to apply NIRS or related methods to precision agriculture domain
Idea: to apply NIRS or related methods for RS data

Question (1): Does NIRS work within 6 bands?
Answer (1): Yes

(Ben-Dor E., and A. Banin, 1995c, Quantitative analysis of convolved TM spectra of soils in the visible, near infrared and short-wave infrared spectral regions (0.4-2.5mm). International Journal of Remote Sensing 18:3509-3528).

Question (2): Does TM- NIRS work?
Answer (2): Yes

Question (1)  

**NIRS in 6 TM bands**

Quantitative analysis of TM spectra of soils

**CaCO₃ (%)**

<table>
<thead>
<tr>
<th>N</th>
<th>R²</th>
<th>SEP</th>
</tr>
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<tbody>
<tr>
<td>50</td>
<td>0.79</td>
<td>11.57</td>
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</tbody>
</table>

**SiO₂ (%)**

<table>
<thead>
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<th>N</th>
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<th>SEP</th>
</tr>
</thead>
<tbody>
<tr>
<td>55</td>
<td>0.88</td>
<td>13.3</td>
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</table>

**Predicted**

**LOI (%)**

<table>
<thead>
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<th>N</th>
<th>R²</th>
<th>SEP</th>
</tr>
</thead>
<tbody>
<tr>
<td>47</td>
<td>0.69</td>
<td>11.4</td>
</tr>
</tbody>
</table>

**SSA (m² g⁻¹)**

<table>
<thead>
<tr>
<th>N</th>
<th>R²</th>
<th>SEP</th>
</tr>
</thead>
<tbody>
<tr>
<td>55</td>
<td>0.67</td>
<td>12.6</td>
</tr>
</tbody>
</table>

**Measured**

Ben-Dor E. and A. Banin, 1995, Quantitative analysis of convolved TM spectra of soils in the visible, near infrared and short-wave infrared spectral regions (0.4-2.5mm). *International Journal of Remote Sensing*, 18:3509-3528.

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Soil Mapping from Orbit using TM

Landsat-5, TM

High iron and clay contents

Low iron and sandy soil

Nanni and Demattê (2005)

Spectral curves

High intensity variation

Loss intensity variation

Question (2)
Idea: to apply NIRS or related methods for HRS data

**Question (3)**: Does NIRS work within real IS data?

**Answer (3)**: Yes


**Question (4)**: Is it straight forward?

**Answer (4)**: No
Question (3)  **NIRS on IS (1)**

*Ben-Dor et al., 2004*
Question (3)

NIRS on IS (2)

Ben-Dor et al., 2004

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Why it is not (yet) straight forward?

- Atmospheric attenuation: requires perfect removal of atmospheric chromophors
  

- Signal to Noise: NIRS requires high SNR data base
  
  (Kruse F.A. Comparison of AVIRIS and Hyperion for Hyperspectral Mineral Mapping In proceedings 11th JPL Airborne Geoscience Workshop, 4-8 March 2002, Pasadena, CA, Jet Propulsion Laboratory Publication 03)

- Subsurface detection: Still problematic, Requires supplementation from other methods
  
  (Heller D., and Ben-Dor E. 2006, A Novel Method of Classifying Soil Profiles in the Field Using Optical Mean Soil Science Society of American Journal)
Quantitative IS of soil properties

- Soil Salinity: (gypsum, sodium)
- Soil properties: (iron oxides, organic matter, clay, carbonates)
- Soil infiltration: (crust, classes)
- Soil Formation: (clay, iron oxides)
- Soil Contamination: (heavy metals)
- Soil Moisture: (H2O)
Soil Salinity (1)

Dehaan and Taylor 2003
Soil Salinity (2)

Ben-Dor et al., 2004

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Soil Formation

Iron oxides as indicator for soil formation

Ben-Dor et al., 2005

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Soil Infiltration and Erosion: Physical Crust (1)

2.2um

1.7um

Clay Accumulation

Particle Size Changes

0 joule

650 joule

1842 joule

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Soil Infiltration and Erosion: Physical Crust (2)

Ben-Dor et al., 2004
Soil Erosion

Map of four soil degradation (erosion) classes derived from AVIRIS data over S-France (I: undisturbed, II: slightly degraded, III: severely degraded - classes IV and V refer to exposed bedrock of marls and limestone) (after Hill et al., 1995).
Soil Toposequence (from field spectroscopy)

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Soil Properties

Figura 1. Gráficos de correlação linear entre os valores determinados em laboratório (VD) e os estimados pelas equações de regressão múltipla (VE) para os atributos do solo.

Gonçalves et al. (2005)
Soil mapping from field spectroscopy

Detailed soil map constructed by traditional methods

Detailed soil map constructed by aerial photographs and spectral radiometry data
Soil Age

Cruvi et al., 2006

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Soil Contamination


- Arsenic Contamination
  - 0 As [ppm] 370
- Lead Contamination
  - 0 Pb [ppm] 2500
- Residual Sludge
  - 0 Weight [g/kg] 140
- Potential Acidification Risk
  - 0 H2SO4 [g/kg] 120
- Calcite-Buffering Need
  - 0 CaCO3 [g/kg] 90

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Swelling Soil

Chabrillat and Goetz, 1999, 2006
Chabrillat et al., 2002
Goetz et al., 2001

Reflectance, %
Wavelength, nm

Smectite
Kaolinite
Smectite/Illite

Smectite
Illite/Smectite
Kaolinite
No clay

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Soil Moisture

Water is significant chromophors
Soil Clay (*Montmorillonite*) and Relative Humidity

Ben-Dor et al 1999
Clayey Soil and Soil Moisture

Bowers and Hanks, 1965

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Inverted Gaussian function is fitted to the fundamental water absorption center at 2800 nm to the convex hull boundary points of a logarithmic transformed SWIR region

Whiting et al., 2004
Soil Water content

Water Content
Red <1%
Green <2%
Blue <5%
Yellow <10%
Cyan <15%
Magenta <20%
Sea Green <32%
Purple >32%
Black = Vegetated or No Data

Whiting (unpublished results)
Soil Water content

Haubrock et al., 2006b
Merge with other remote sensing technique

Surface Gypsum Correlated with 60 cm depth EC

\[ y = 0.3568x - 1.98 \]

\[ R^2 = 0.9566 \]

Field Spectroscopy

Salinity as an Example
State of Science of Environmental Application of Imaging Spectroscopy in honor of Prof. A. Goetz

Salinity as an Example
Soil map production

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Vision: IS should be commercially and economically operated (rather than only scientifically used)

Example: NIRS

Commercially Covers: food, textile, tobacco, pharmacological, medicine, vegetation, soil and more….
Near Infrared Spectroscopy: Time for the Giant to Wake Up!

A. M. C. Davies, AFRC Institute of Food Research, Norwich Laboratory, Colney Lane, Norwich NR4 7UA, UK

Introduction

A few years ago Professor David Wieland described near infrared (NIR) analysis as a “sleeping technique”. Although since that article there has been no discernible increase in the use of NIR methods of analysis, what has been happening is a continual widening of the base of potential applications of NIR analysis. It is becoming increasingly evident that NIR will make considerable contributions to many areas of analysis of major importance in the 1990s. One of the signs of this confidence among NIR spectroscopists is the formation of an International Committee for Near Infrared Spectroscopy (ICNIRS) at a meeting in Budapest last May. The first conference under the auspices of the ICNIRS will be held at the University of East Anglia, Norwich, UK, 12-17 July 1987 where it will form part of the Spectroscopy Across the Spectrum: Analytical Applications of Spectroscopy conference.

In this article, I will review the theory of NIR spectroscopy and the basic steps in the development of an NIR method, look at some of the more recent applications, outline some of the improved methods of data analysis and discuss what is limiting the development of NIR analysis.

NIR Theory

Absorption bands in the near infrared region of the electromagnetic spectrum are caused by overtones or combinations of fundamental absorptions occurring in the mid-infrared region. It has become the accepted convention that peak positions in NIR spectra are expressed in terms of wavelength measured in nm. As most spectra are obtained by reflectance measurements, the absorbance is normally expressed as log I/I₀ where I₀ is the reflectance. There is no satisfactory justification for the use of log I/I₀, but experiments have demonstrated that other models, such as Kubelka-Munk, do not give improved results. When measurements are obtained in the transmission mode then log (I/I₀) is used and Beer’s Law can be applied.

Figure 1. Near infrared spectra of aqueous ethanol solutions (0-100% water) obtained in a transmission cell fitted to a Perkin Elmer 6830 Mark I NIR spectrometer. The inset is an expansion of the region from 1950-2000 nm showing selected absorptions of the ethanol and water. The NIR region is divided into three sub-bands: the alcohol band at 1900-1940 nm.

Figure 2. Diffuse reflectance near infrared spectra are affected by particulate variations. Spectra are of the same sample of tea, immersed in deionised water for 15 minutes, with the concentration varying from 1 to 50 mg/l. The particle size distribution of the sample is shown in the inset. The spectra are affected by the presence of more intense absorption bands from other constituents, as illustrated in Fig. 1. The analysis is based on the differences in particle size distribution, as demonstrated in Fig. 2.

As NIR absorptions are related to IR absorptions there is a similar relationship between bond strength, molecular mass and peak position but in NIR spectroscopy there is considerable overlap because of the multiplicity of overtones and combinations. Absorption bands in the NIR region are much weaker than those in the IR region and this is an important factor which facilitates the analytical application of NIR. For example, in the IR region diffuse reflection PIR measurements often require dilution of the sample, this is generally not required for NIR measurements. It can be obtained that NIR absorption bands are not obscured by the presence of more intense absorption bands from other constituents, as illustrated in Fig. 1. The analysis is based on the differences in particle size distribution, as demonstrated in Fig. 2.

Near infrared absorptions are not dependent on the particle size distribution, which is an advantage in the analysis of particulate matter. The NIR spectra can be used to determine the concentration of the analyte in the sample, provided that the analyte concentration is above the detection limit. The analysis is based on the differences in particle size distribution, as demonstrated in Fig. 2.
The history of near infrared spectroscopic analysis: Past, present and future – “From sleeping technique to the morning star of spectroscopy”

T. Davies

Norwich Near Infrared Consultancy, 75 Intwood Road, Cringleford, Norwich, NR4 6AA, UK

The history of the analytical use of near infrared (NIR) spectroscopy is reviewed and its future potential is assessed. This future is very bright if sufficient new researchers are attracted to this academically unfashionable spectroscopy.

“Glittering like the Morning Star, full of life, splendour and joy”

Edmund Burke, 1790.

important as a stepping stone to the rest of the electromagnetic spectrum. There was a brief period of interest in the late 19th century, which can be summarised by the work of Abney and Festing [5] and then in the 1950’s there was rather more interest, which has been recounted by Whetsel [6,7].
Vision (1)

A paper based on this presentation submitted to the special issue of:


..........By means of this paper, we will have the privilege of making the entire soil science community aware of this important field and saying: “(Soil) Imaging Analysis: Time for the Giant Wake up Call”.

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NIRS-IS similarities

NIRS
• 1968- Ben-Gera and Norrish (first paper)
• 1987- Davies paper (let the giant...)
• 2000- Commercially operated

IS
• 1984- Van and Goetz (first paper)
• 2006-Ben-Dor’s paper (let the giant..)
• 2010- Commercially operated
Conclusion remarks

• The Imaging Spectroscopy has reached a point of no return....

• Imaging Spectroscopy in the soil environment has a bright future.....

• Commercializing Imaging spectroscopy for soil and other applications may be a key for success....

• A new Journal covering Imaging Spectroscopy applications (such as NIRJ for NIRS) is missing: We suggest to establish a new journal entitled: Journal of Imaging Spectroscopy
We thank Alex for opening the IS window for the scientific community and hope to see in IGARSS 2015 >20% of the sessions - IS oriented.....

We thank all of you for your attention