Soil Spectroscopy: Principle and Applications

Novospec

THE REMOTE SENSING LABORATORIES

Prof. Eyal Ben Dor

Department of Geography and Human Environment

Brno Czech Republic, June 25-26

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Quantitative Soil Spectral Analysis

Lesson 4

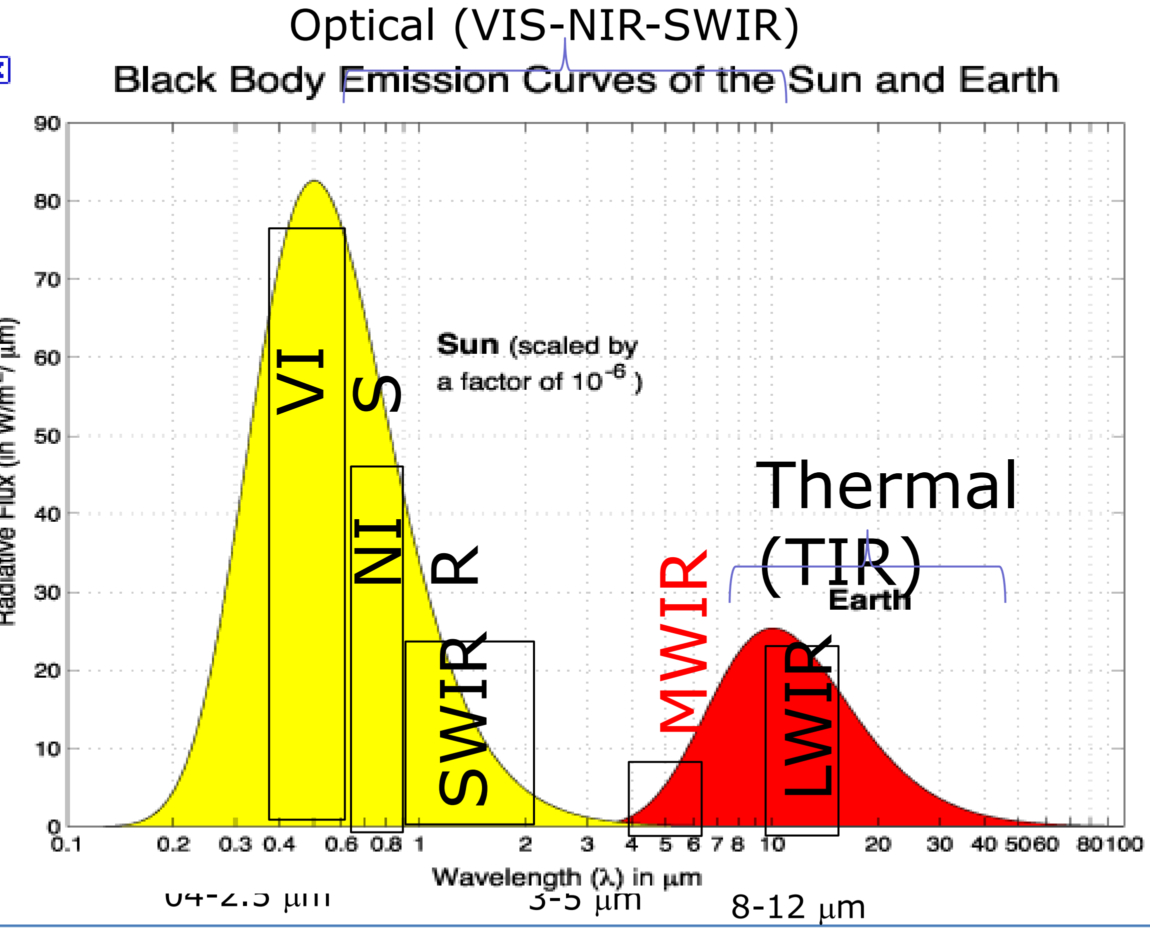
Terminology :

Near infra-red spectroscopy (NIRS)
Near Infrared Analysis (NIRA)
vis-NIR

All are based first on the 1000-2500nm spectral region (termed as NIR by food sceinsts).

Problem with the term : **vis-NIR**

Radiation Sources, Atmosphere Windows and available Detectors create the well accepted (and logical) jargon in the (Hyperspectral) Remote Sensing Community



VIS- Visible (0.4-0.7um)

NIR- Near InfarRed (0.7-1.0 um)

SWIR- Short Wav Infrared (1.0-2.5um)

MWIR- Middle Wave Infrared (2.5-5um)

LWIR- Lower Wave Infrared (8-12um)

Non of these terms, as well as the vis-NIR reflects what we are realy doing: chmometrics based on (reflectance) spectroscopy

As we measure Reflectance and do Spectral Analysis the correct term should be :

SpeR - A (Spectral Reflectance - Analysis). It can be done in the VNIR-SWIR, in the VNIR or in the SWIR

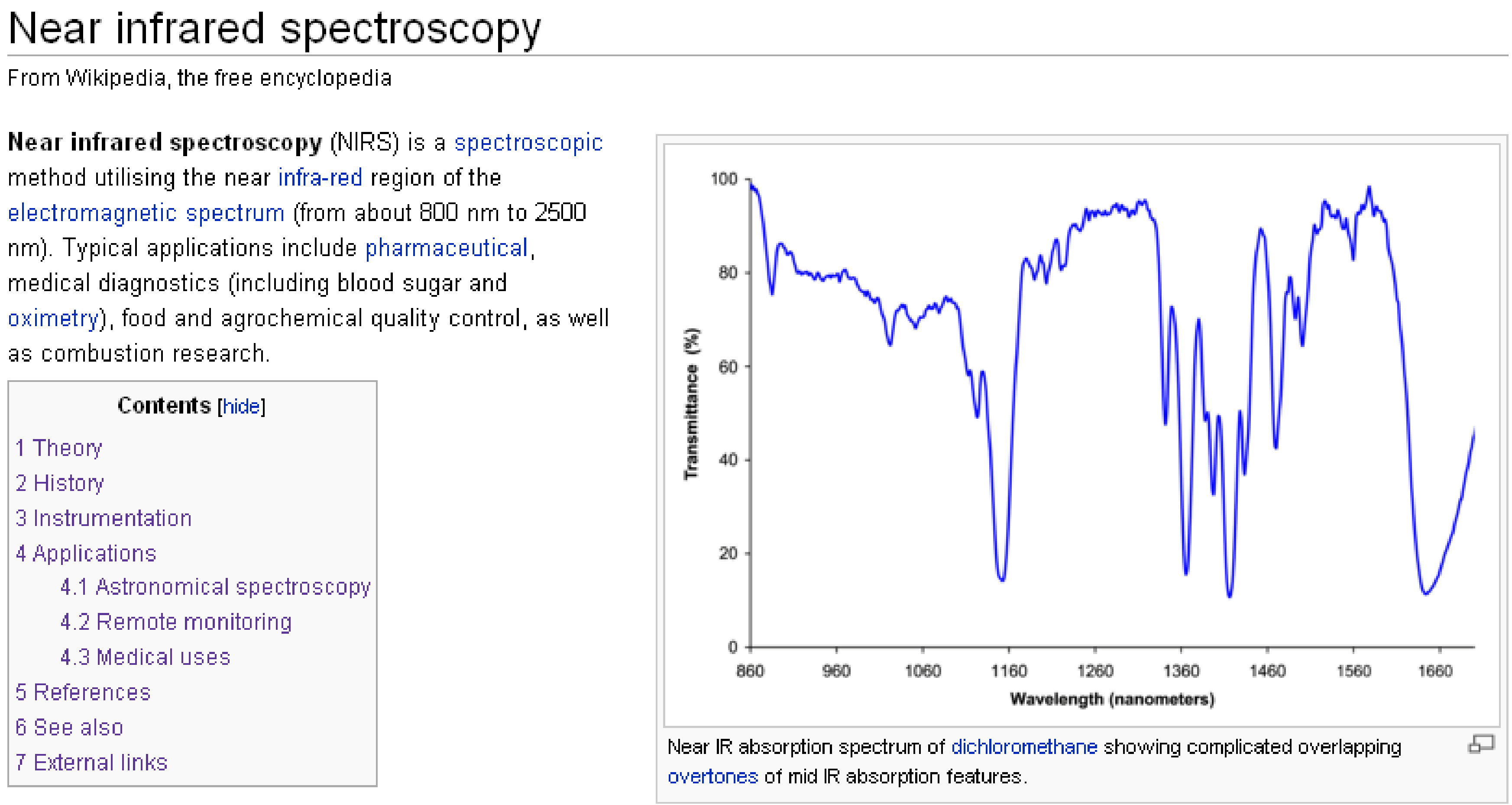
It is also a **spare** method for the wet chemistry

NIR past and present

http://coolcosmos.ipac.caltech.edu/cosmic_classroom/ir_tutorial/discovery.html

The history of near infrared (NIR) begins in 1800 with **Frederick William Herschel.**

He was trying filters to observe sun spots and when he used a red one, he noticed that a lot of heat was produced, which was of a higher temperature than the visible spectrum. After further studying, he concluded that there must be an invisible form of light beyond the visible spectrum.



Near infrared spectroscopy

From Wikipedia, the free encyclopedia

Near infrared spectroscopy (NIRS) is a spectroscopic method utilising the near infra-red region of the electromagnetic spectrum (from about 800 nm to 2500 nm). Typical applications include pharmaceutical, medical diagnostics (including blood sugar and oximetry), food and agrochemical quality control, as well as combustion research.

Contents [hide]

Near IR absorption spectrum of dichloromethane showing complicated overlapping overtones of mid IR absorption features.

What is NIRS ?

- **Near infra-red (NIR) spectroscopy is a technology that exploits the NIR spectral region by finding a model between laboratory measures and reflectance information**

- **It evolved in 1968 by Norris and Ben Gera**

(*Determination of moisture content in soybeans by direct Israel. J. Agric. Res, 125-132*)

- **The NIRS was first covered the 1000-2500nm but today it is covering also the VIS (400-700nm), NIR (700-1000nm) and SWIR (short infrared) (1000-2500nm).**
- **The term NIRS – still exists but the spectral regions are different from its origin.**

NIRS is used today in many disciplines such as: agriculture, medicine, tobacco industry, Pharmacology, paper industry, geology….and soil science.

As the NIRS is a part of natural sunlight , it is also implemented in the to HSR dicipline: Starting with and Vegetation recently also with soils

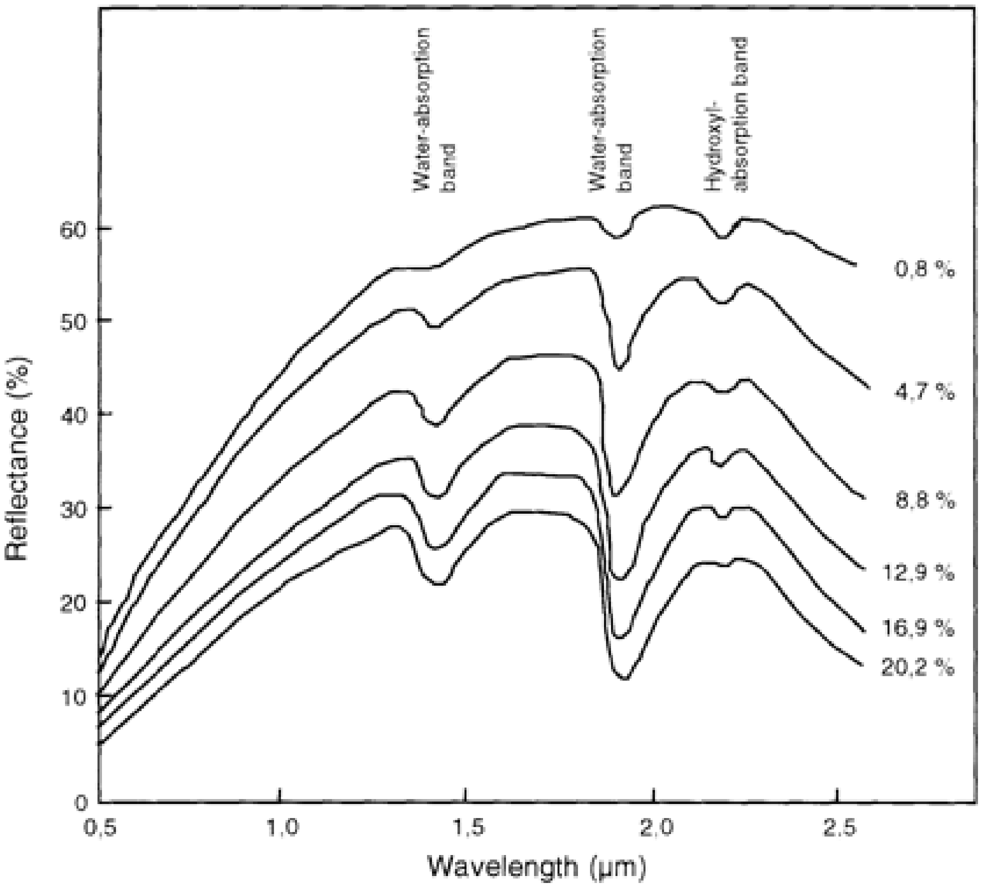
(*Wessman, C.A., Aber, J.D., Peterson, D.L., & Melillo, J.M. (1988) Remote sensing of canopy chemistry and nitrogen cycling in temperate forest ecosystems. Nature, 335, 154.*)

***Ben-Dor, E., K. Patkin, A. Banin, and A. Karnieli. 2002. Mapping of several soil properties using DAIS-7915 hyperspectral scanner data. A case study over clayey soils in Israel. Int. J. Remote Sens. 23:1043–1062.*)**

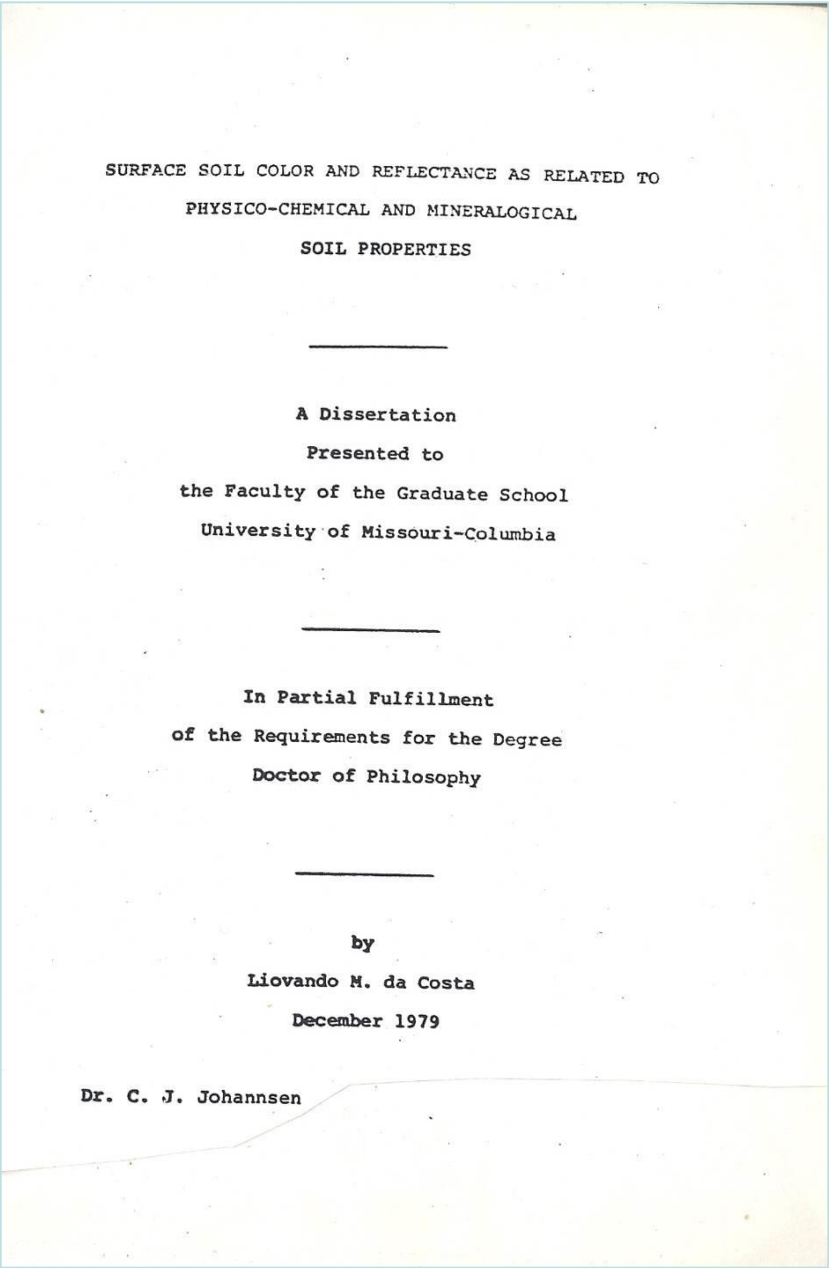
Quantitative Soil Spectroscopy :
Some Mile stones (a personal view)

1968 Ben Gera and Norris – **first NIRS paper on grains**
1970 Condit – **Soil Moisture interaction – a quantitative view**
1979 De Costa **– First PhD on quantitative soil spectroscopy**
1980 -1 Stoner and Baumgardner – **First Soil Atlas,**
First Spectra classification
1986 Dalal and Henry – **First NIRS soil paper (SM, N,C**)
1991 ASD - **First (real) portable spectrometer**
1994-5 Ben-Dor and Banin **– Elaboration of the NIRS to featureless**
Properties
1988 Davies **– First NIRS workshop**
1993 Batten **– First NIRS Journal**
2002 Ben-Dor et al- **First NIRS work on soil from IS domain**
2006 Viscarra Rossel - **A summary of many NIRS works**
2008 Visscara Rossel – **Soil World Spectral Library**
2010 Spectral Tool (POS) **- A spectral accessory to measure soil profile**
(commercial applications are available)
2011 HYSPRI **- soil spectral library request**

Condit, H.R. 1970. The spectral reflectance of American Soils. Photogramme Engg. V. 36, pp. 955–966.



1970



SURFACE SOIL COLOR AND REFLECTANCE AS RELATED TO
PHYSICO-CHEMICAL AND MINERALOGICAL
SOIL PROPERTIES

A Dissertation
Presented to
the Faculty of the Graduate School
University of Missouri-Columbia

In Partial Fulfillment
of the Requirements for the Degree
Doctor of Philosophy

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by
Liovando M. da Costa
December 1979

Dr. C. J. Johannsen

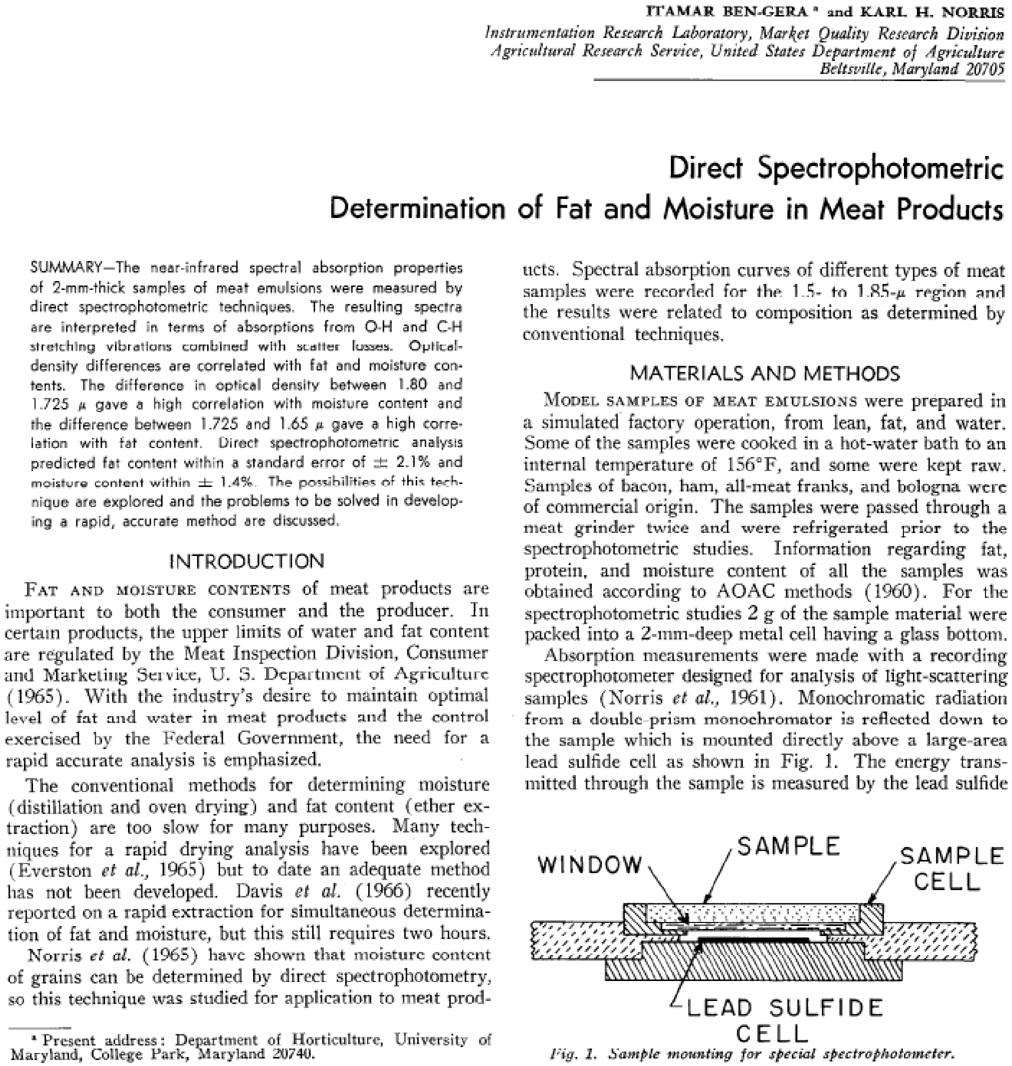
1979

First PhD on Soil Spectroscopy and quantitative approach

University of Minnesota

De Costa

1969
Ben Gera and Norrish



ITAMAR BEN-GERA[a] and **KARL H. NORRIS**
Instrumentation Research Laboratory, Market Quality Research Division
Agricultural Research Service, United States Department of Agriculture
Beltsville, Maryland 20705

Direct Spectrophotometric Determination of Fat and Moisture in Meat Products

SUMMARY—The near-infrared spectral absorption properties of 2-mm-thick samples of meat emulsions were measured by direct spectrophotometric techniques. The resulting spectra are interpreted in terms of absorptions from O-H and C-H stretching vibrations combined with scatter losses. Optical-density differences are correlated with fat and moisture contents. The difference in optical density between 1.80 and 1.725 μ gave a high correlation with moisture content and the difference between 1.725 and 1.65 μ gave a high correlation with fat content. Direct spectrophotometric analysis predicted fat content within a standard error of ± 2.1% and moisture content within ± 1.4%. The possibilities of this technique are explored and the problems to be solved in developing a rapid, accurate method are discussed.

INTRODUCTION

FAT AND MOISTURE CONTENTS of meat products are important to both the consumer and the producer. In certain products, the upper limits of water and fat content are regulated by the Meat Inspection Division, Consumer and Marketing Service, U. S. Department of Agriculture (1965). With the industry's desire to maintain optimal level of fat and water in meat products and the control exercised by the Federal Government, the need for a rapid accurate analysis is emphasized.

The conventional methods for determining moisture (distillation and oven drying) and fat content (ether extraction) are too slow for many purposes. Many techniques for a rapid drying analysis have been explored (Everston *et al.*, 1965) but to date an adequate method has not been developed. Davis *et al.* (1966) recently reported on a rapid extraction for simultaneous determination of fat and moisture, but this still requires two hours.

Norris *et al.* (1965) have shown that moisture content of grains can be determined by direct spectrophotometry, so this technique was studied for application to meat products. Spectral absorption curves of different types of meat samples were recorded for the 1.5- to 1.85-μ region and the results were related to composition as determined by conventional techniques.

MATERIALS AND METHODS

MODEL SAMPLES OF MEAT EMULSIONS were prepared in a simulated factory operation, from lean, fat, and water. Some of the samples were cooked in a hot-water bath to an internal temperature of 156°F, and some were kept raw. Samples of bacon, ham, all-meat franks, and bologna were of commercial origin. The samples were passed through a meat grinder twice and were refrigerated prior to the spectrophotometric studies. Information regarding fat, protein, and moisture content of all the samples was obtained according to AOAC methods (1960). For the spectrophotometric studies 2 g of the sample material were packed into a 2-mm-deep metal cell having a glass bottom.

Absorption measurements were made with a recording spectrophotometer designed for analysis of light-scattering samples (Norris *et al.*, 1961). Monochromatic radiation from a double-prism monochromator is reflected down to the sample which is mounted directly above a large-area lead sulfide cell as shown in Fig. 1. The energy transmitted through the sample is measured by the lead sulfide

Fig. 1. Sample mounting for special spectrophotometer.

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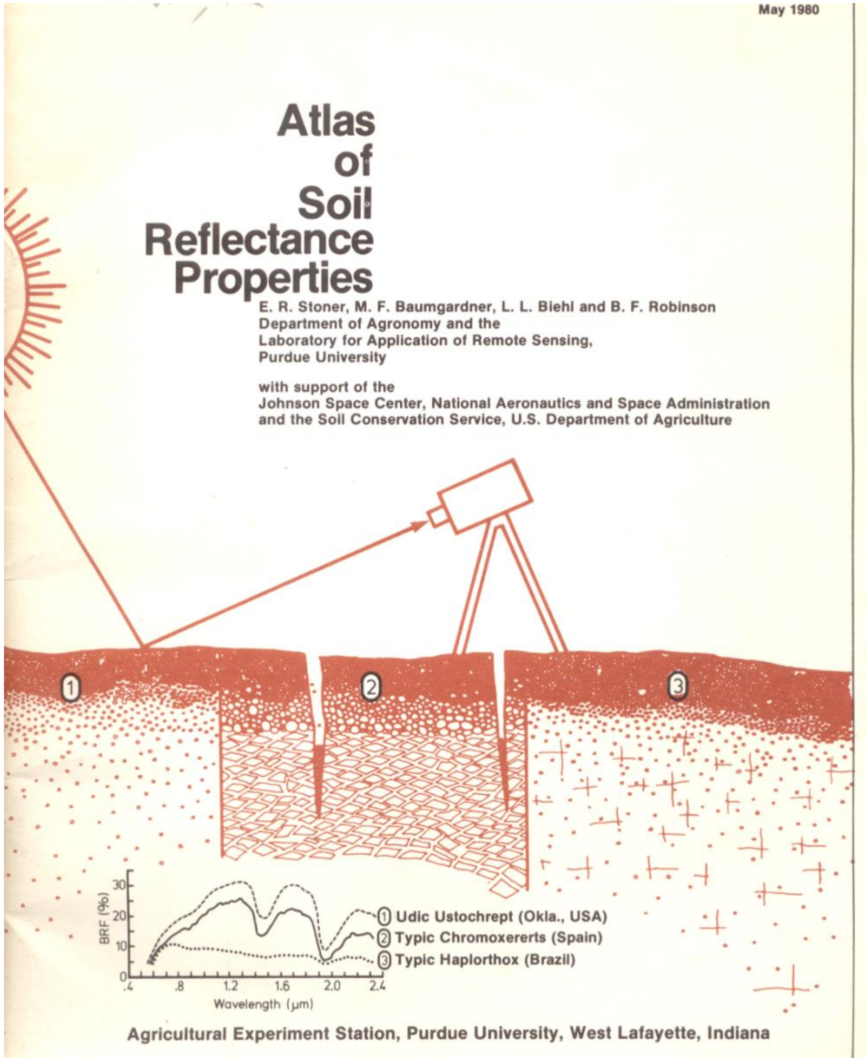
[a] Present address: Department of Horticulture, University of Maryland, College Park, Maryland 20740.

Stoner, E. R., Baumgardner, M. F., Biehl, L. L., and Robinson, B. F. 1980. “Atlas of soil reflectance properties , laboratory for application of Remote Sensing,” Purdue University Research Bulletin 962.



May 1980

Atlas of Soil Reflectance Properties

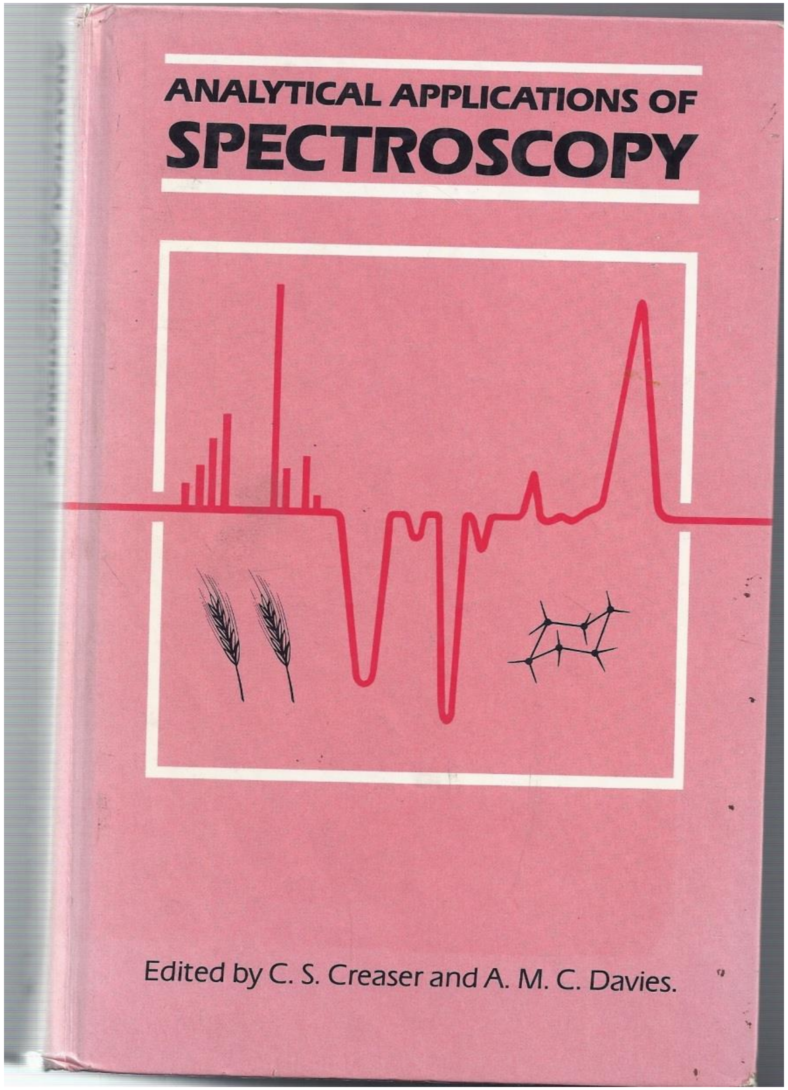
E. R. Stoner, M. F. Baumgardner, L. L. Biehl and B. F. Robinson
Department of Agronomy and the
Laboratory for Application of Remote Sensing,
Purdue University

with support of the
Johnson Space Center, National Aeronautics and Space Administration
and the Soil Conservation Service, U.S. Department of Agriculture

① Udic Ustochrept (Okla., USA)
② Typic Chromoxererts (Spain)
③ Typic Haplorthox (Brazil)

Agricultural Experiment Station, Purdue University, West Lafayette, Indiana

1980

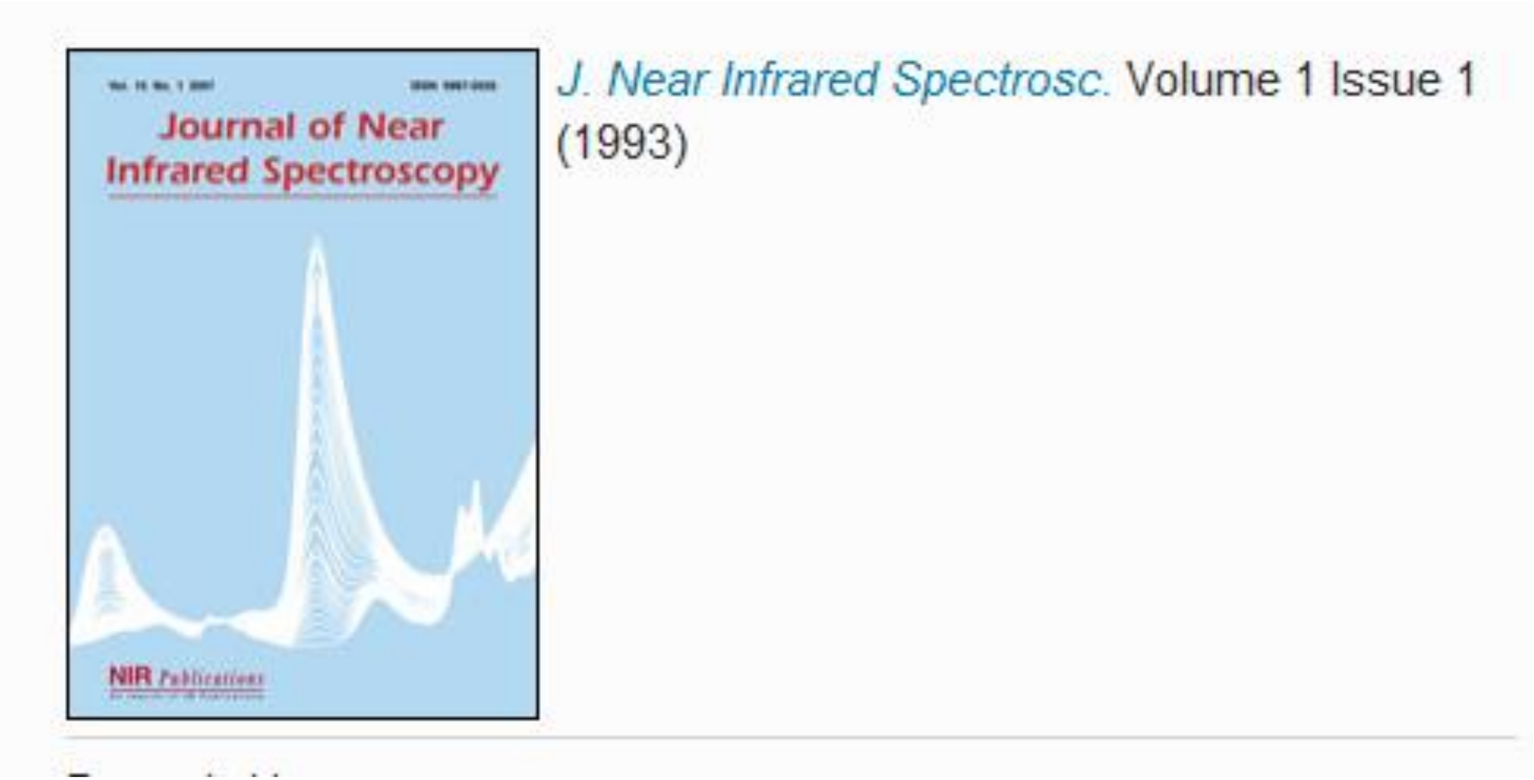


ANALYTICAL APPLICATIONS OF
SPECTROSCOPY

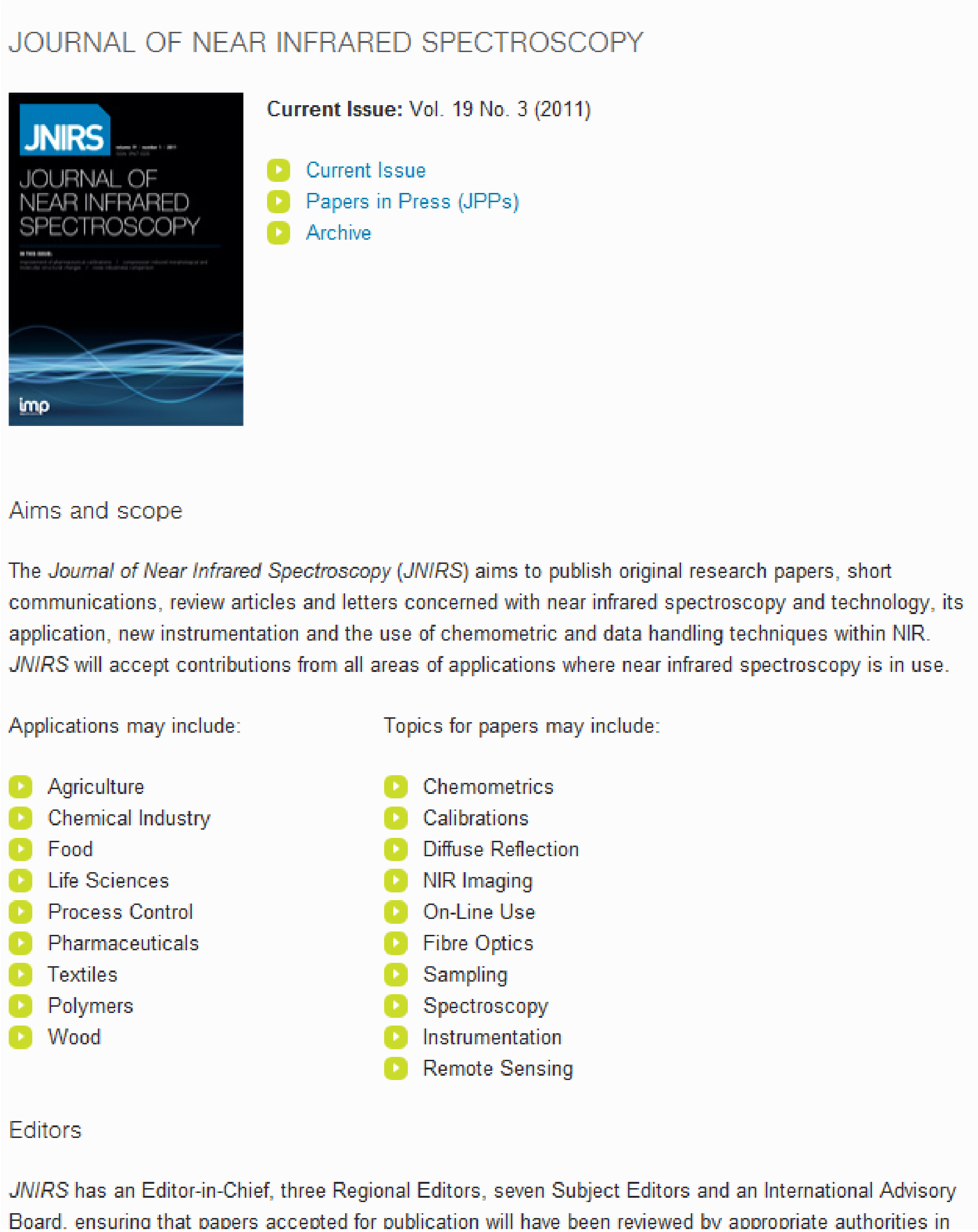
Edited by C. S. Creaser and A. M. C. Davies.

1988

First Conference
in NIRS



J. Near Infrared Spectrosc. Volume 1 Issue 1 (1993)



JOURNAL OF NEAR INFRARED SPECTROSCOPY

Current Issue: Vol. 19 No. 3 (2011)

- Current Issue
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Aims and scope

The *Journal of Near Infrared Spectroscopy* (*JNIRS*) aims to publish original research papers, short communications, review articles and letters concerned with near infrared spectroscopy and technology, its application, new instrumentation and the use of chemometric and data handling techniques within NIR. *JNIRS* will accept contributions from all areas of applications where near infrared spectroscopy is in use.

Applications may include:

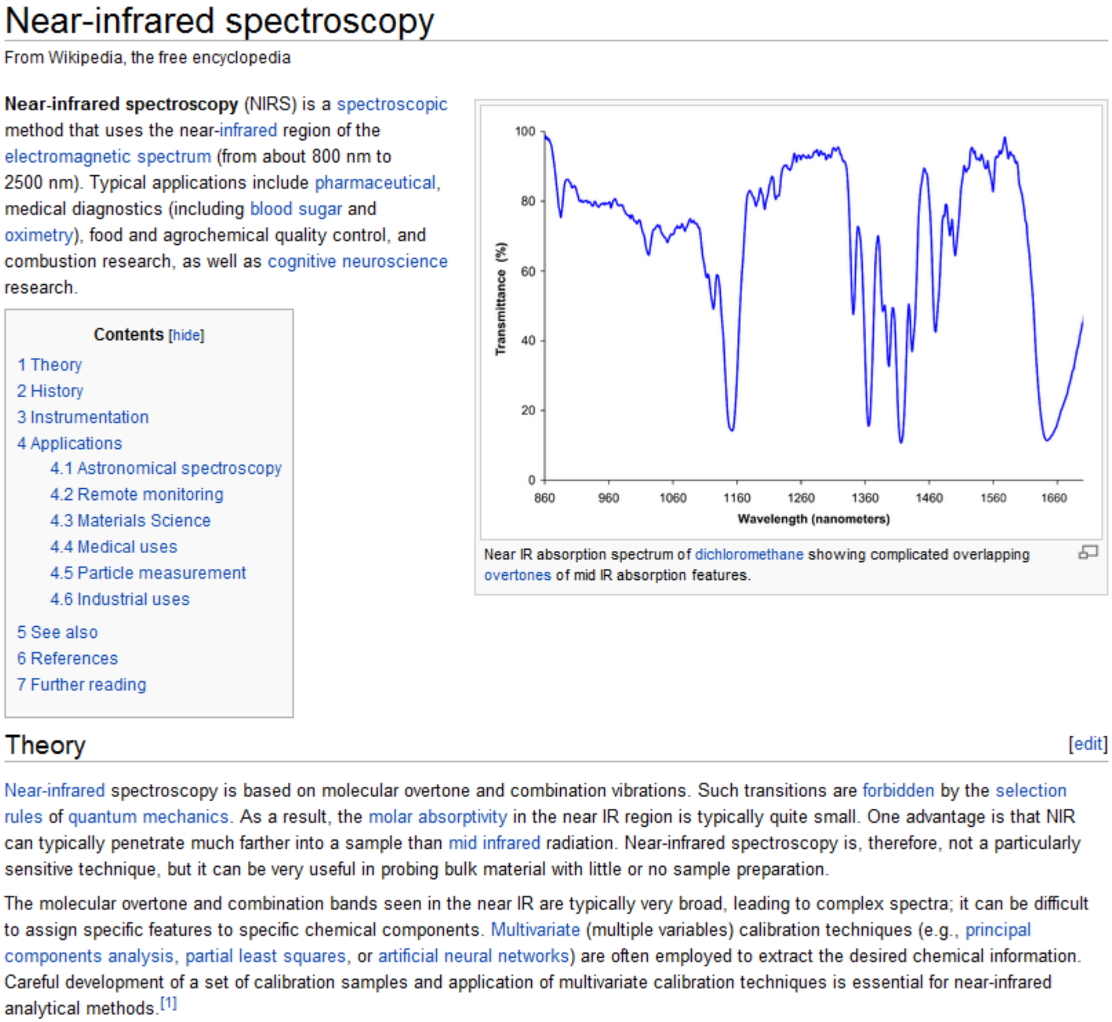
- Agriculture
- Chemical Industry
- Food
- Life Sciences
- Process Control
- Pharmaceuticals
- Textiles
- Polymers
- Wood

Topics for papers may include:

- Chemometrics
- Calibrations
- Diffuse Reflection
- NIR Imaging
- On-Line Use
- Fibre Optics
- Sampling
- Spectroscopy
- Instrumentation
- Remote Sensing

Editors

JNIRS has an Editor-in-Chief, three Regional Editors, seven Subject Editors and an International Advisory Board, ensuring that papers accepted for publication will have been reviewed by appropriate authorities in



Near-infrared spectroscopy

From Wikipedia, the free encyclopedia

Near-infrared spectroscopy (NIRS) is a spectroscopic method that uses the near-infrared region of the electromagnetic spectrum (from about 800 nm to 2500 nm). Typical applications include pharmaceutical, medical diagnostics (including blood sugar and oximetry), food and agrochemical quality control, and combustion research, as well as cognitive neuroscience research.

Near IR absorption spectrum of dichloromethane showing complicated overlapping overtones of mid IR absorption features.

Contents [hide]

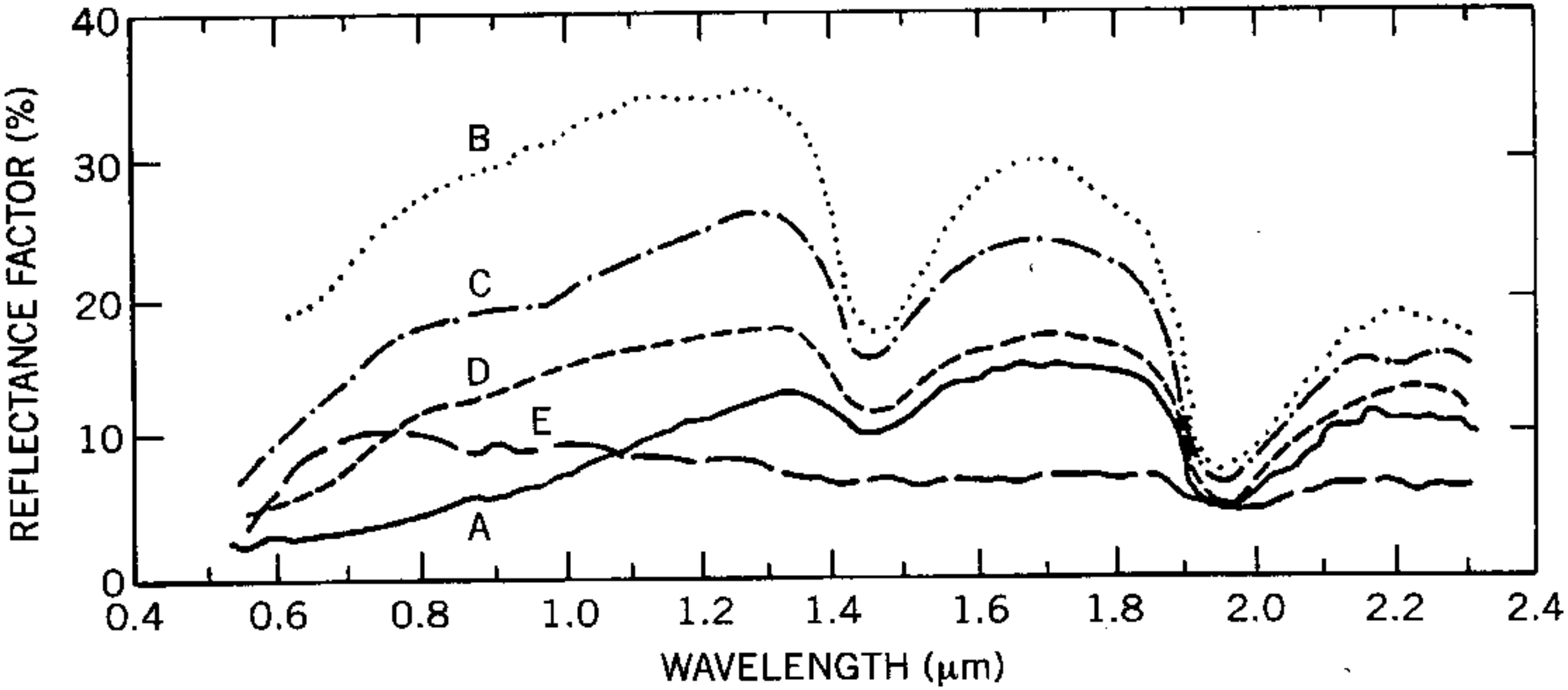
Theory

[edit]

Near-infrared spectroscopy is based on molecular overtone and combination vibrations. Such transitions are forbidden by the selection rules of quantum mechanics. As a result, the molar absorptivity in the near IR region is typically quite small. One advantage is that NIR can typically penetrate much farther into a sample than mid infrared radiation. Near-infrared spectroscopy is, therefore, not a particularly sensitive technique, but it can be very useful in probing bulk material with little or no sample preparation.

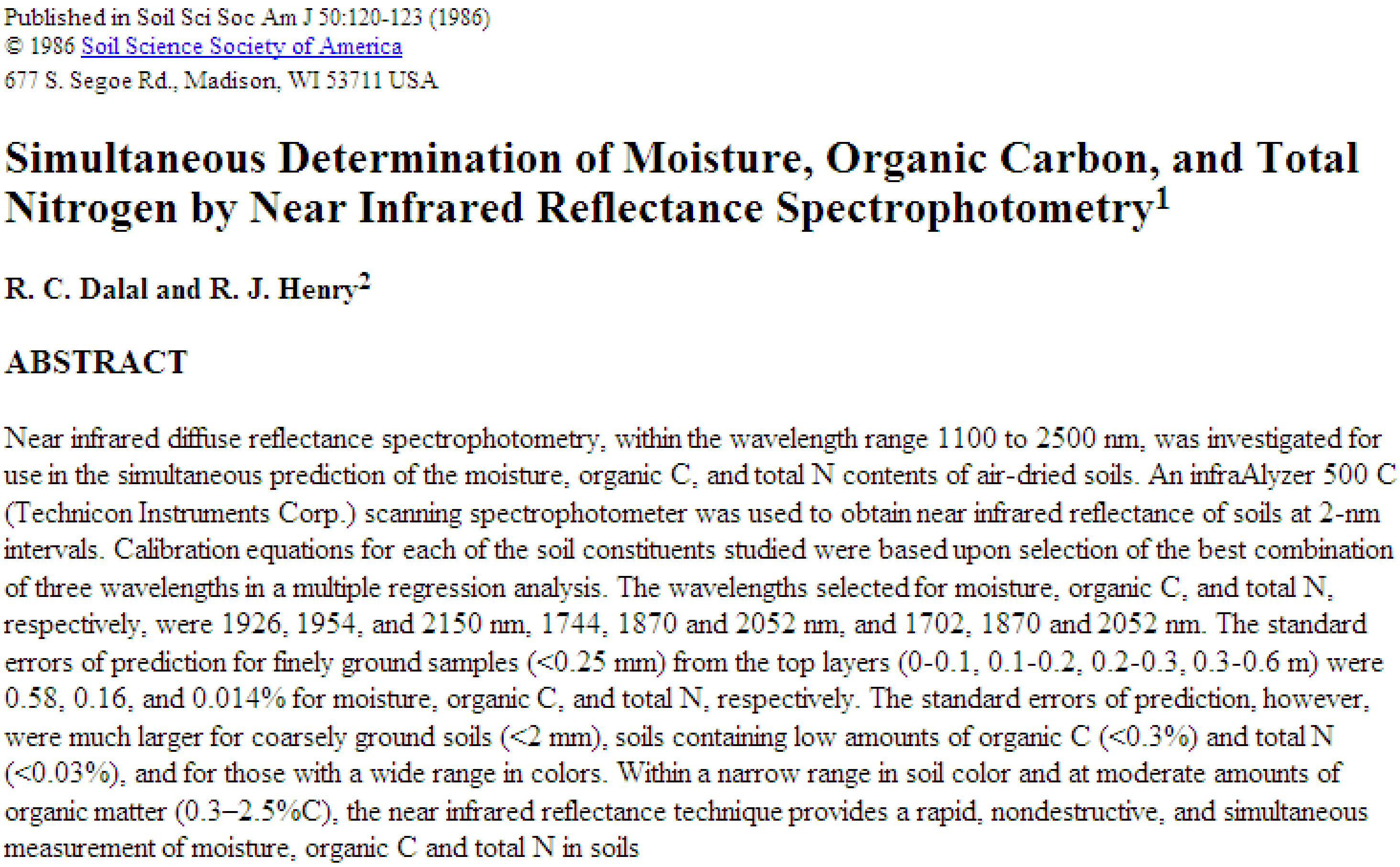
The molecular overtone and combination bands seen in the near IR are typically very broad, leading to complex spectra; it can be difficult to assign specific features to specific chemical components. Multivariate (multiple variables) calibration techniques (e.g., principal components analysis, partial least squares, or artificial neural networks) are often employed to extract the desired chemical information. Careful development of a set of calibration samples and application of multivariate calibration techniques is essential for near-infrared analytical methods.[1]

Stoner, E.R., & Baumgardner, M.F. 1981. Characteristic Variation in reflectance of surface soils. Soil Sci. Soc. Am. J.V. 45, 1161–1165.



1981

R. C. Dalal and R. J. Henry 1986 Simultaneous Determination of Moisture, Organic Carbon, and Total Nitrogen by Near Infrared Reflectance Spectrophotometry Soil Sci Soc Am J 50:120-123



Published in Soil Sci Soc Am J 50:120-123 (1986)
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677 S. Segoe Rd., Madison, WI 53711 USA

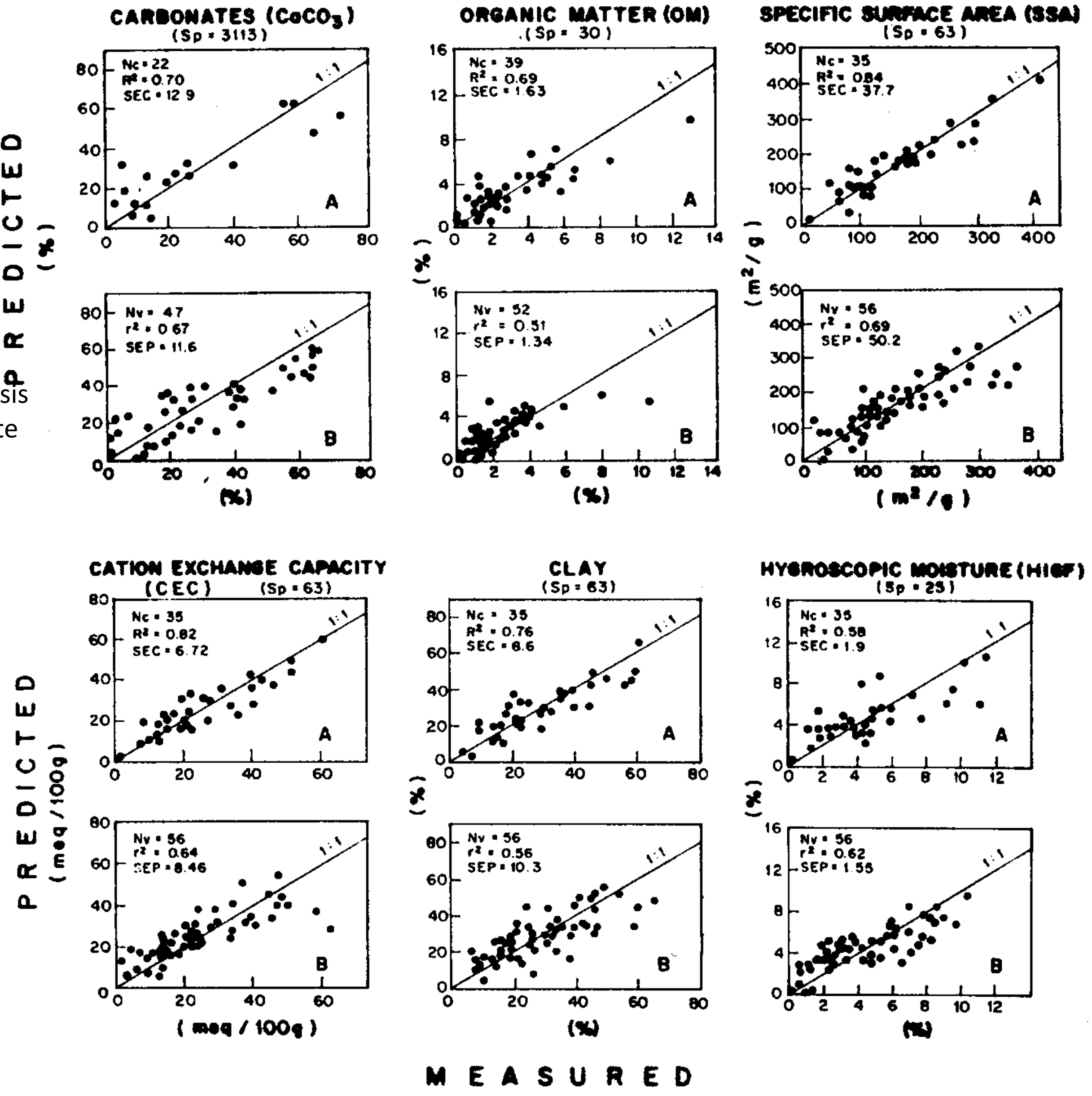
Simultaneous Determination of Moisture, Organic Carbon, and Total Nitrogen by Near Infrared Reflectance Spectrophotometry[1]

R. C. Dalal and R. J. Henry[2]

ABSTRACT

Near infrared diffuse reflectance spectrophotometry, within the wavelength range 1100 to 2500 nm, was investigated for use in the simultaneous prediction of the moisture, organic C, and total N contents of air-dried soils. An infraAlyzer 500 C (Technicon Instruments Corp.) scanning spectrophotometer was used to obtain near infrared reflectance of soils at 2-nm intervals. Calibration equations for each of the soil constituents studied were based upon selection of the best combination of three wavelengths in a multiple regression analysis. The wavelengths selected for moisture, organic C, and total N, respectively, were 1926, 1954, and 2150 nm, 1744, 1870 and 2052 nm, and 1702, 1870 and 2052 nm. The standard errors of prediction for finely ground samples (<0.25 mm) from the top layers (0-0.1, 0.1-0.2, 0.2-0.3, 0.3-0.6 m) were 0.58, 0.16, and 0.014% for moisture, organic C, and total N, respectively. The standard errors of prediction, however, were much larger for coarsely ground soils (<2 mm), soils containing low amounts of organic C (<0.3%) and total N (<0.03%), and for those with a wide range in colors. Within a narrow range in soil color and at moderate amounts of organic matter (0.3–2.5%C), the near infrared reflectance technique provides a rapid, nondestructive, and simultaneous measurement of moisture, organic C and total N in soils

1986



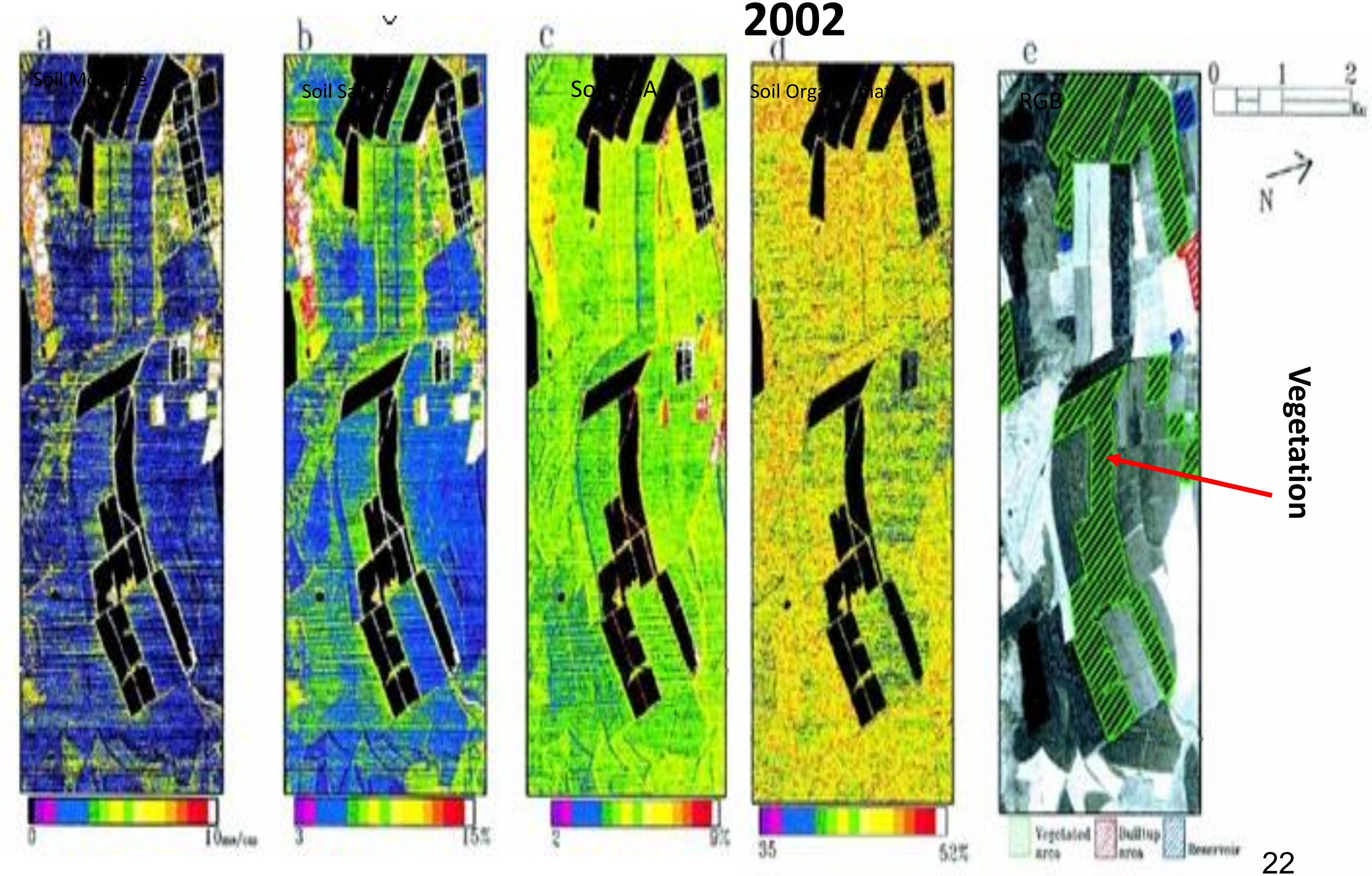
Ben-Dor E. and A. Banin 1995, Near infrared analysis (NIRA) as a simultaneously method to evaluate spectral featureless constituents in oils., *Soil Science,159:259-268* 159:259-269

Ben-Dor E., and A. Banin, 1994, Visible and near infrared (0.4-1.1µm) analysis of arid and semi arid soils. *Remote Sensing of Environment,* 48:261-274

1994-5

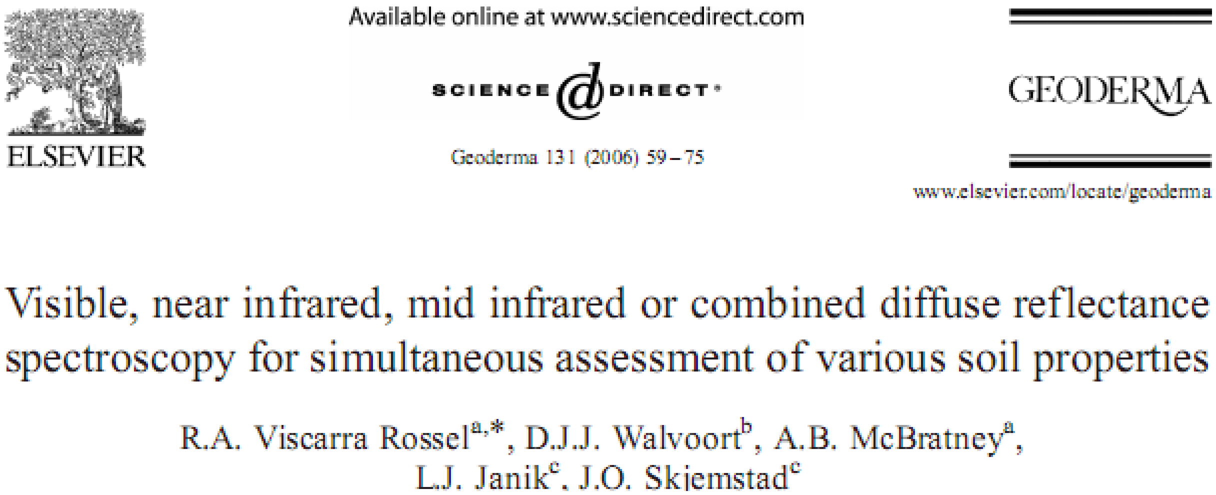
Ben-Dor E., K. Patkin, A. Banin and A. Karnieli 2002 Mapping of several soil properties using DAIS-7915 hyperspectral scanner data. A case study over clayey soils in Israel. International Journal of Remote Sensing 23:1043-1062.

2002



Vegetation

NIRS in soil



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Geoderma 131 (2006) 59 – 75

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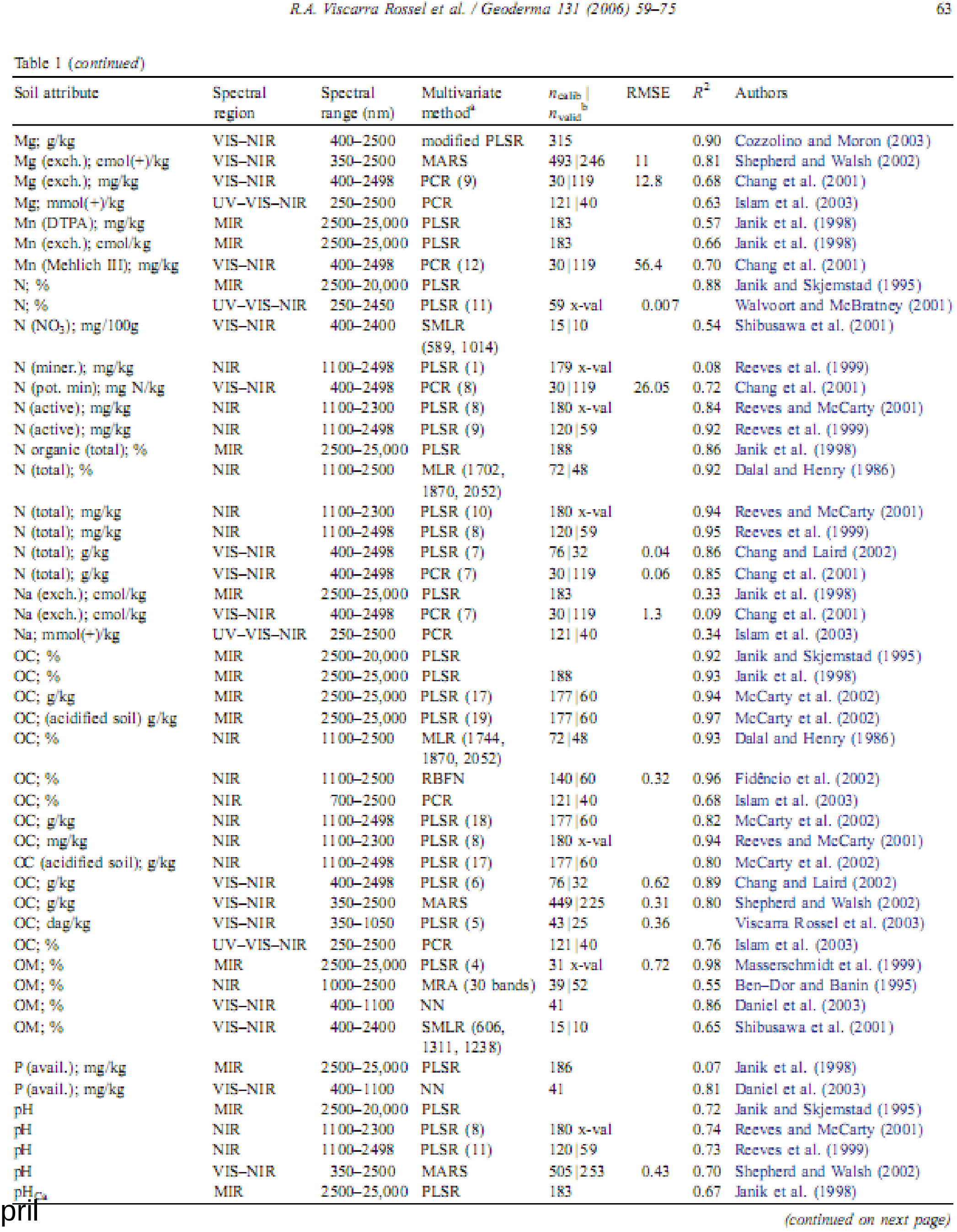
Visible, near infrared, mid infrared or combined diffuse reflectance spectroscopy for simultaneous assessment of various soil properties

R.A. Viscarra Rossel[a,*], D.J.J. Walvoort[b], A.B. McBratney[a],
L.J. Janik[c], J.O. Skjemstad[c]

2006



R.A. Viscarra Rossel et al. / Geoderma 131 (2006) 59–75 63

Table 1 (*continued*)

Soil attribute	Spectral region	Spectral range (nm)	Multivariate method[a]	n_{calib} | n_{valid}[b]	RMSE	R^2	Authors
Mg; g/kg	VIS–NIR	400–2500	modified PLSR	315		0.90	Cozzolino and Moron (2003)
Mg (exch.); cmol(+)/kg	VIS–NIR	350–2500	MARS	493 | 246	11	0.81	Shepherd and Walsh (2002)
Mg (exch.); mg/kg	VIS–NIR	400–2498	PCR (9)	30 | 119	12.8	0.68	Chang et al. (2001)
Mg; mmol(+)/kg	UV–VIS–NIR	250–2500	PCR	121 | 40		0.63	Islam et al. (2003)
Mn (DTPA); mg/kg	MIR	2500–25,000	PLSR	183		0.57	Janik et al. (1998)
Mn (exch.); cmol/kg	MIR	2500–25,000	PLSR	183		0.66	Janik et al. (1998)
Mn (Mehlich III); mg/kg	VIS–NIR	400–2498	PCR (12)	30 | 119	56.4	0.70	Chang et al. (2001)
N; %	MIR	2500–20,000	PLSR			0.88	Janik and Skjemstad (1995)
N; %	UV–VIS–NIR	250–2450	PLSR (11)	59 x-val	0.007		Walvoort and McBratney (2001)
N (NO_3); mg/100g	VIS–NIR	400–2400	SMLR (589, 1014)	15 | 10		0.54	Shibusawa et al. (2001)
N (miner.); mg/kg	NIR	1100–2498	PLSR (1)	179 x-val		0.08	Reeves et al. (1999)
N (pot. min); mg N/kg	VIS–NIR	400–2498	PCR (8)	30 | 119	26.05	0.72	Chang et al. (2001)
N (active); mg/kg	NIR	1100–2300	PLSR (8)	180 x-val		0.84	Reeves and McCarty (2001)
N (active); mg/kg	NIR	1100–2498	PLSR (9)	120 | 59		0.92	Reeves et al. (1999)
N organic (total); %	MIR	2500–25,000	PLSR	188		0.86	Janik et al. (1998)
N (total); %	NIR	1100–2500	MLR (1702, 1870, 2052)	72 | 48		0.92	Dalal and Henry (1986)
N (total); mg/kg	NIR	1100–2300	PLSR (10)	180 x-val		0.94	Reeves and McCarty (2001)
N (total); mg/kg	NIR	1100–2498	PLSR (8)	120 | 59		0.95	Reeves et al. (1999)
N (total); g/kg	VIS–NIR	400–2498	PLSR (7)	76 | 32	0.04	0.86	Chang and Laird (2002)
N (total); g/kg	VIS–NIR	400–2498	PCR (7)	30 | 119	0.06	0.85	Chang et al. (2001)
Na (exch.); cmol/kg	MIR	2500–25,000	PLSR	183		0.33	Janik et al. (1998)
Na (exch.); cmol/kg	VIS–NIR	400–2498	PCR (7)	30 | 119	1.3	0.09	Chang et al. (2001)
Na; mmol(+)/kg	UV–VIS–NIR	250–2500	PCR	121 | 40		0.34	Islam et al. (2003)
OC; %	MIR	2500–20,000	PLSR			0.92	Janik and Skjemstad (1995)
OC; %	MIR	2500–25,000	PLSR	188		0.93	Janik et al. (1998)
OC; g/kg	MIR	2500–25,000	PLSR (17)	177 | 60		0.94	McCarty et al. (2002)
OC; (acidified soil) g/kg	MIR	2500–25,000	PLSR (19)	177 | 60		0.97	McCarty et al. (2002)
OC; %	NIR	1100–2500	MLR (1744, 1870, 2052)	72 | 48		0.93	Dalal and Henry (1986)
OC; %	NIR	1100–2500	RBFN	140 | 60	0.32	0.96	Fidêncio et al. (2002)
OC; %	NIR	700–2500	PCR	121 | 40		0.68	Islam et al. (2003)
OC; g/kg	NIR	1100–2498	PLSR (18)	177 | 60		0.82	McCarty et al. (2002)
OC; mg/kg	NIR	1100–2300	PLSR (8)	180 x-val		0.94	Reeves and McCarty (2001)
OC (acidified soil); g/kg	NIR	1100–2498	PLSR (17)	177 | 60		0.80	McCarty et al. (2002)
OC; g/kg	VIS–NIR	400–2498	PLSR (6)	76 | 32	0.62	0.89	Chang and Laird (2002)
OC; g/kg	VIS–NIR	350–2500	MARS	449 | 225	0.31	0.80	Shepherd and Walsh (2002)
OC; dag/kg	VIS–NIR	350–1050	PLSR (5)	43 | 25	0.36		Viscarra Rossel et al. (2003)
OC; %	UV–VIS–NIR	250–2500	PCR	121 | 40		0.76	Islam et al. (2003)
OM; %	MIR	2500–25,000	PLSR (4)	31 x-val	0.72	0.98	Masserschmidt et al. (1999)
OM; %	NIR	1000–2500	MRA (30 bands)	39 | 52		0.55	Ben-Dor and Banin (1995)
OM; %	VIS–NIR	400–1100	NN	41		0.86	Daniel et al. (2003)
OM; %	VIS–NIR	400–2400	SMLR (606, 1311, 1238)	15 | 10		0.65	Shibusawa et al. (2001)
P (avail.); mg/kg	MIR	2500–25,000	PLSR	186		0.07	Janik et al. (1998)
P (avail.); mg/kg	VIS–NIR	400–1100	NN	41		0.81	Daniel et al. (2003)
pH	MIR	2500–20,000	PLSR			0.72	Janik and Skjemstad (1995)
pH	NIR	1100–2300	PLSR (8)	180 x-val		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_{Ca}	MIR	2500–25,000	PLSR	183		0.67	Janik et al. (1998)

(*continued on next page*)

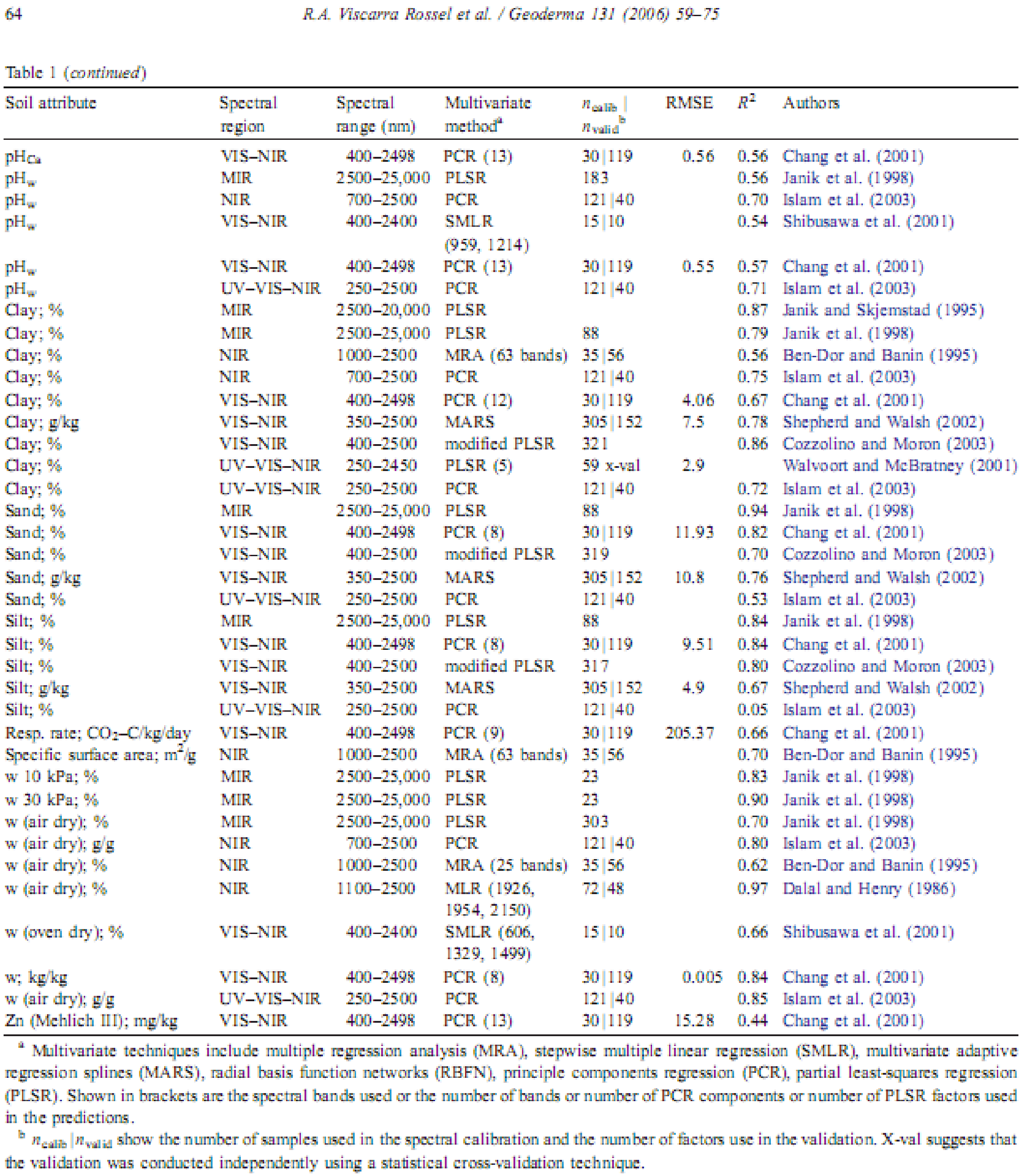


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Table 1 (*continued*)

Soil attribute	Spectral region	Spectral range (nm)	Multivariate method[a]	n_{calib} | n_{valid}[b]	RMSE	R^2	Authors
pH_{Ca}	VIS–NIR	400–2498	PCR (13)	30 | 119	0.56	0.56	Chang et al. (2001)
pH_w	MIR	2500–25,000	PLSR	183		0.56	Janik et al. (1998)
pH_w	NIR	700–2500	PCR	121 | 40		0.70	Islam et al. (2003)
pH_w	VIS–NIR	400–2400	SMLR (959, 1214)	15 | 10		0.54	Shibusawa et al. (2001)
pH_w	VIS–NIR	400–2498	PCR (13)	30 | 119	0.55	0.57	Chang et al. (2001)
pH_w	UV–VIS–NIR	250–2500	PCR	121 | 40		0.71	Islam et al. (2003)
Clay; %	MIR	2500–20,000	PLSR			0.87	Janik and Skjemstad (1995)
Clay; %	MIR	2500–25,000	PLSR	88		0.79	Janik et al. (1998)
Clay; %	NIR	1000–2500	MRA (63 bands)	35 | 56		0.56	Ben-Dor and Banin (1995)
Clay; %	NIR	700–2500	PCR	121 | 40		0.75	Islam et al. (2003)
Clay; %	VIS–NIR	400–2498	PCR (12)	30 | 119	4.06	0.67	Chang et al. (2001)
Clay; g/kg	VIS–NIR	350–2500	MARS	305 | 152	7.5	0.78	Shepherd and Walsh (2002)
Clay; %	VIS–NIR	400–2500	modified PLSR	321		0.86	Cozzolino and Moron (2003)
Clay; %	UV–VIS–NIR	250–2450	PLSR (5)	59 x-val	2.9		Walvoort and McBratney (2001)
Clay; %	UV–VIS–NIR	250–2500	PCR	121 | 40		0.72	Islam et al. (2003)
Sand; %	MIR	2500–25,000	PLSR	88		0.94	Janik et al. (1998)
Sand; %	VIS–NIR	400–2498	PCR (8)	30 | 119	11.93	0.82	Chang et al. (2001)
Sand; %	VIS–NIR	400–2500	modified PLSR	319		0.70	Cozzolino and Moron (2003)
Sand; g/kg	VIS–NIR	350–2500	MARS	305 | 152	10.8	0.76	Shepherd and Walsh (2002)
Sand; %	UV–VIS–NIR	250–2500	PCR	121 | 40		0.53	Islam et al. (2003)
Silt; %	MIR	2500–25,000	PLSR	88		0.84	Janik et al. (1998)
Silt; %	VIS–NIR	400–2498	PCR (8)	30 | 119	9.51	0.84	Chang et al. (2001)
Silt; %	VIS–NIR	400–2500	modified PLSR	317		0.80	Cozzolino and Moron (2003)
Silt; g/kg	VIS–NIR	350–2500	MARS	305 | 152	4.9	0.67	Shepherd and Walsh (2002)
Silt; %	UV–VIS–NIR	250–2500	PCR	121 | 40		0.05	Islam et al. (2003)
Resp. rate; CO_2–C/kg/day	VIS–NIR	400–2498	PCR (9)	30 | 119	205.37	0.66	Chang et al. (2001)
Specific surface area; m^2/g	NIR	1000–2500	MRA (63 bands)	35 | 56		0.70	Ben-Dor and Banin (1995)
w 10 kPa; %	MIR	2500–25,000	PLSR	23		0.83	Janik et al. (1998)
w 30 kPa; %	MIR	2500–25,000	PLSR	23		0.90	Janik et al. (1998)
w (air dry); %	MIR	2500–25,000	PLSR	303		0.70	Janik et al. (1998)
w (air dry); g/g	NIR	700–2500	PCR	121 | 40		0.80	Islam et al. (2003)
w (air dry); %	NIR	1000–2500	MRA (25 bands)	35 | 56		0.62	Ben-Dor and Banin (1995)
w (air dry); %	NIR	1100–2500	MLR (1926, 1954, 2150)	72 | 48		0.97	Dalal and Henry (1986)
w (oven dry); %	VIS–NIR	400–2400	SMLR (606, 1329, 1499)	15 | 10		0.66	Shibusawa et al. (2001)
w; kg/kg	VIS–NIR	400–2498	PCR (8)	30 | 119	0.005	0.84	Chang et al. (2001)
w (air dry); g/g	UV–VIS–NIR	250–2500	PCR	121 | 40		0.85	Islam et al. (2003)
Zn (Mehlich III); mg/kg	VIS–NIR	400–2498	PCR (13)	30 | 119	15.28	0.44	Chang et al. (2001)

[a] Multivariate techniques include multiple regression analysis (MRA), stepwise multiple linear regression (SMLR), multivariate adaptive regression splines (MARS), radial basis function networks (RBFN), principle components regression (PCR), partial least-squares regression (PLSR). Shown in brackets are the spectral bands used or the number of bands or number of PCR components or number of PLSR factors used in the predictions.

[b] n_{calib} | n_{valid} show the number of samples used in the spectral calibration and the number of factors use in the validation. X-val suggests that the validation was conducted independently using a statistical cross-validation technique.

Example from Viscarra Rossel list (1

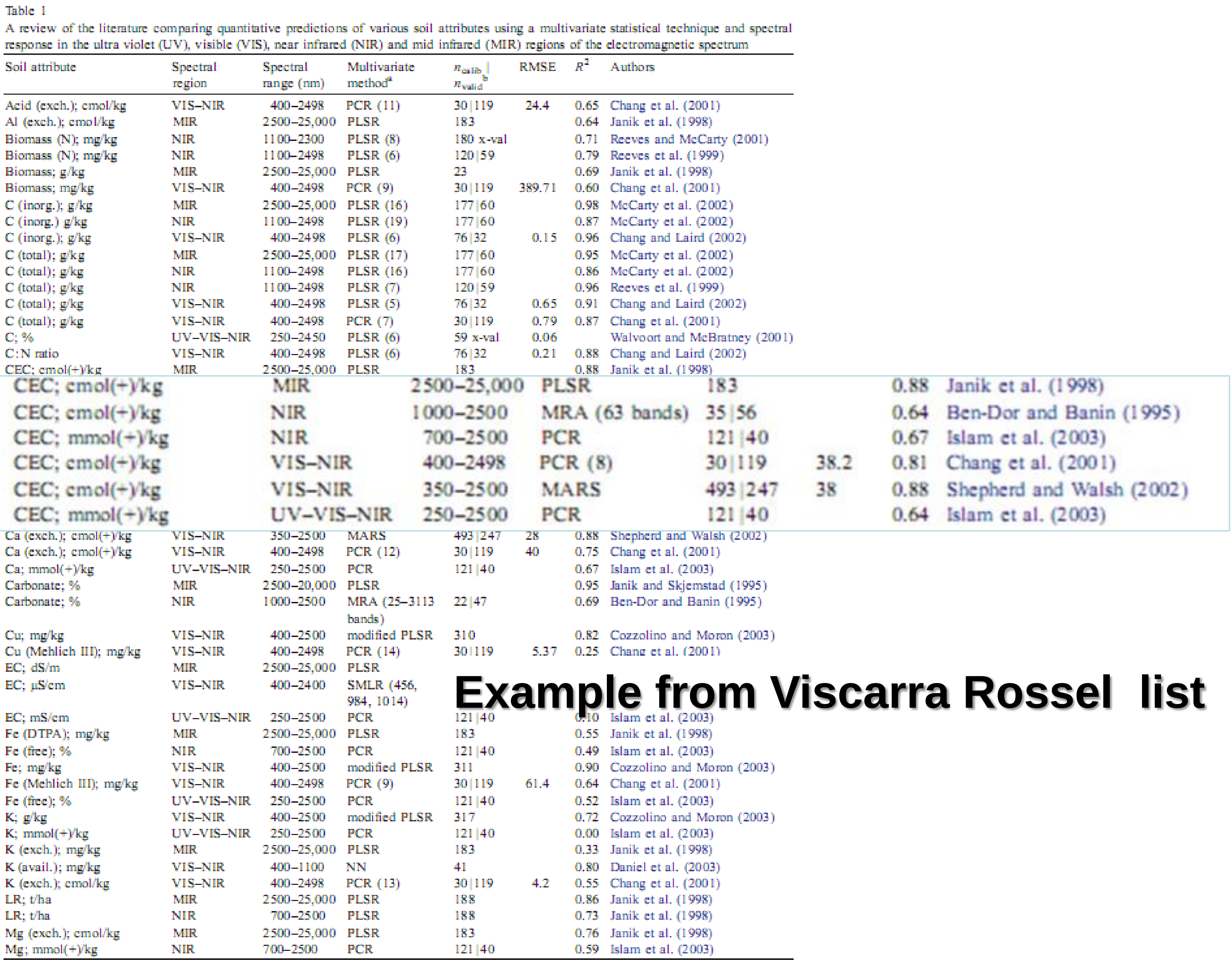
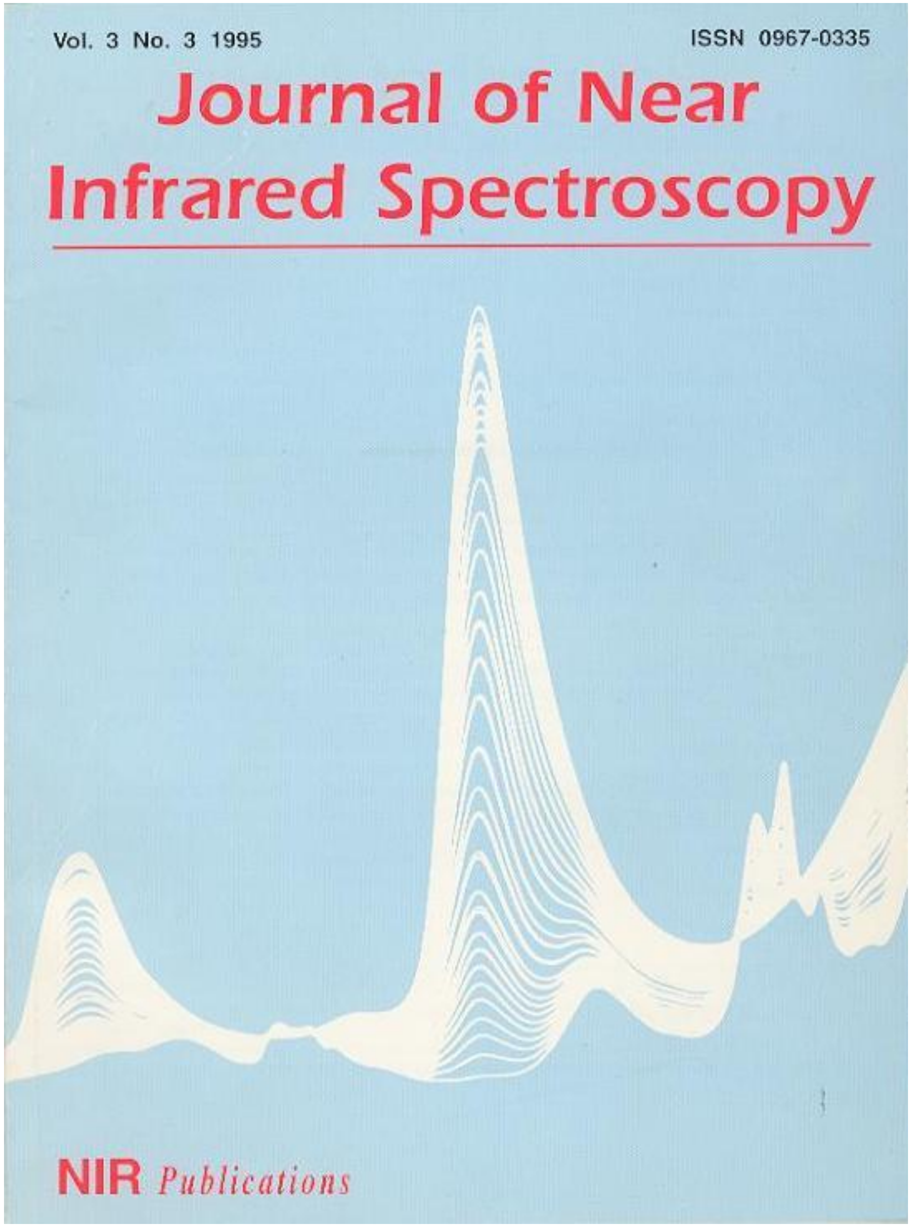


Table 1

A review of the literature comparing quantitative predictions of various soil attributes using a multivariate statistical technique and spectral response in the ultra violet (UV), visible (VIS), near infrared (NIR) and mid infrared (MIR) regions of the electromagnetic spectrum

Soil attribute	Spectral region	Spectral range (nm)	Multivariate method[a]	n_{calib} | n_{valid}[b]	RMSE	R^2	Authors
Acid (exch.); cmol/kg	VIS–NIR	400–2498	PCR (11)	30|119	24.4	0.65	Chang et al. (2001)
Al (exch.); cmol/kg	MIR	2500–25,000	PLSR	183		0.64	Janik et al. (1998)
Biomass (N); mg/kg	NIR	1100–2300	PLSR (8)	180 x-val		0.71	Reeves and McCarty (2001)
Biomass (N); mg/kg	NIR	1100–2498	PLSR (6)	120|59		0.79	Reeves et al. (1999)
Biomass; g/kg	MIR	2500–25,000	PLSR	23		0.69	Janik et al. (1998)
Biomass; mg/kg	VIS–NIR	400–2498	PCR (9)	30|119	389.71	0.60	Chang et al. (2001)
C (inorg.); g/kg	MIR	2500–25,000	PLSR (16)	177|60		0.98	McCarty et al. (2002)
C (inorg.) g/kg	NIR	1100–2498	PLSR (19)	177|60		0.87	McCarty et al. (2002)
C (inorg.); g/kg	VIS–NIR	400–2498	PLSR (6)	76|32	0.15	0.96	Chang and Laird (2002)
C (total); g/kg	MIR	2500–25,000	PLSR (17)	177|60		0.95	McCarty et al. (2002)
C (total); g/kg	NIR	1100–2498	PLSR (16)	177|60		0.86	McCarty et al. (2002)
C (total); g/kg	NIR	1100–2498	PLSR (7)	120|59		0.96	Reeves et al. (1999)
C (total); g/kg	VIS–NIR	400–2498	PLSR (5)	76|32	0.65	0.91	Chang and Laird (2002)
C (total); g/kg	VIS–NIR	400–2498	PCR (7)	30|119	0.79	0.87	Chang et al. (2001)
C; %	UV–VIS–NIR	250–2450	PLSR (6)	59 x-val	0.06		Walvoort and McBratney (2001)
C:N ratio	VIS–NIR	400–2498	PLSR (6)	76|32	0.21	0.88	Chang and Laird (2002)
CEC; cmol(+)/kg	MIR	2500–25,000	PLSR	183		0.88	Janik et al. (1998)
CEC; cmol(+)/kg	MIR	2500–25,000	PLSR	183		0.88	Janik et al. (1998)
CEC; cmol(+)/kg	NIR	1000–2500	MRA (63 bands)	35|56		0.64	Ben-Dor and Banin (1995)
CEC; mmol(+)/kg	NIR	700–2500	PCR	121|40		0.67	Islam et al. (2003)
CEC; cmol(+)/kg	VIS–NIR	400–2498	PCR (8)	30|119	38.2	0.81	Chang et al. (2001)
CEC; cmol(+)/kg	VIS–NIR	350–2500	MARS	493|247	38	0.88	Shepherd and Walsh (2002)
CEC; mmol(+)/kg	UV–VIS–NIR	250–2500	PCR	121|40		0.64	Islam et al. (2003)
Ca (exch.); cmol(+)/kg	VIS–NIR	350–2500	MARS	493|247	28	0.88	Shepherd and Walsh (2002)
Ca (exch.); cmol(+)/kg	VIS–NIR	400–2498	PCR (12)	30|119	40	0.75	Chang et al. (2001)
Ca; mmol(+)/kg	UV–VIS–NIR	250–2500	PCR	121|40		0.67	Islam et al. (2003)
Carbonate; %	MIR	2500–20,000	PLSR			0.95	Janik and Skjemstad (1995)
Carbonate; %	NIR	1000–2500	MRA (25–3113 bands)	22|47		0.69	Ben-Dor and Banin (1995)
Cu; mg/kg	VIS–NIR	400–2500	modified PLSR	310		0.82	Cozzolino and Moron (2003)
Cu (Mehlich III); mg/kg	VIS–NIR	400–2498	PCR (14)	30|119	5.37	0.25	Chang et al. (2001)
EC; dS/m	MIR	2500–25,000	PLSR				
EC; µS/cm	VIS–NIR	400–2400	SMLR (456, 984, 1014)				
EC; mS/cm	UV–VIS–NIR	250–2500	PCR	121|40		0.10	Islam et al. (2003)
Fe (DTPA); mg/kg	MIR	2500–25,000	PLSR	183		0.55	Janik et al. (1998)
Fe (free); %	NIR	700–2500	PCR	121|40		0.49	Islam et al. (2003)
Fe; mg/kg	VIS–NIR	400–2500	modified PLSR	311		0.90	Cozzolino and Moron (2003)
Fe (Mehlich III); mg/kg	VIS–NIR	400–2498	PCR (9)	30|119	61.4	0.64	Chang et al. (2001)
Fe (free); %	UV–VIS–NIR	250–2500	PCR	121|40		0.52	Islam et al. (2003)
K; g/kg	VIS–NIR	400–2500	modified PLSR	317		0.72	Cozzolino and Moron (2003)
K; mmol(+)/kg	UV–VIS–NIR	250–2500	PCR	121|40		0.00	Islam et al. (2003)
K (exch.); mg/kg	MIR	2500–25,000	PLSR	183		0.33	Janik et al. (1998)
K (avail.); mg/kg	VIS–NIR	400–1100	NN	41		0.80	Daniel et al. (2003)
K (exch.); cmol/kg	VIS–NIR	400–2498	PCR (13)	30|119	4.2	0.55	Chang et al. (2001)
LR; t/ha	MIR	2500–25,000	PLSR	188		0.86	Janik et al. (1998)
LR; t/ha	NIR	700–2500	PLSR	188		0.73	Janik et al. (1998)
Mg (exch.); cmol/kg	MIR	2500–25,000	PLSR	183		0.76	Janik et al. (1998)
Mg; mmol(+)/kg	NIR	700–2500	PCR	121|40		0.59	Islam et al. (2003)



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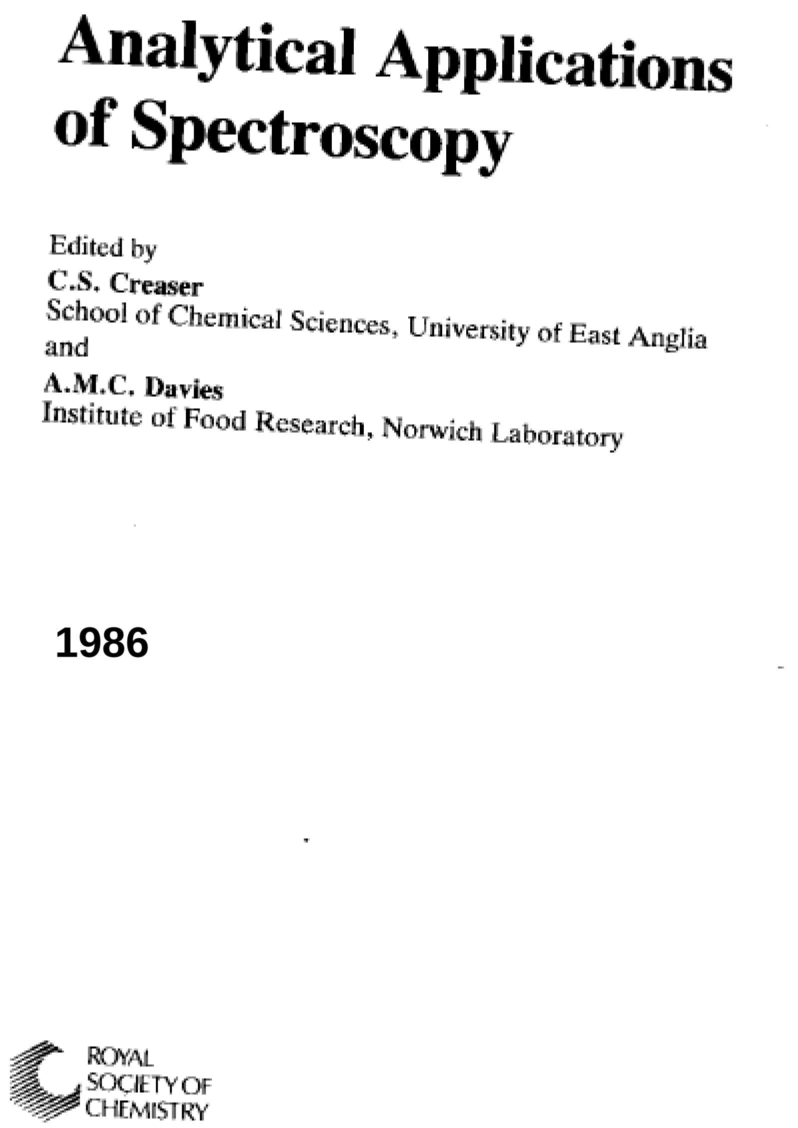

Analytical Applications of Spectroscopy

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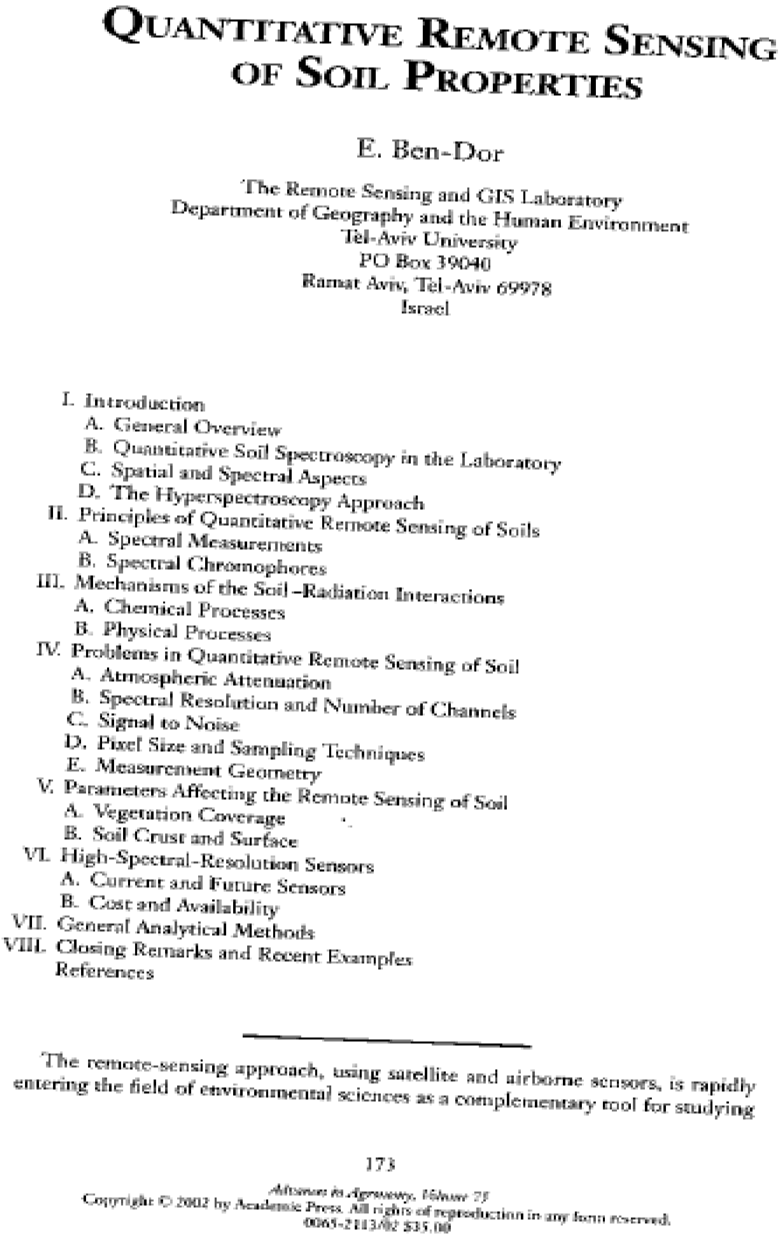
1986

ROYAL SOCIETY OF CHEMISTRY



QUANTITATIVE REMOTE SENSING OF SOIL PROPERTIES

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The remote-sensing approach, using satellite and airborne sensors, is rapidly entering the field of environmental sciences as a complementary tool for studying

173

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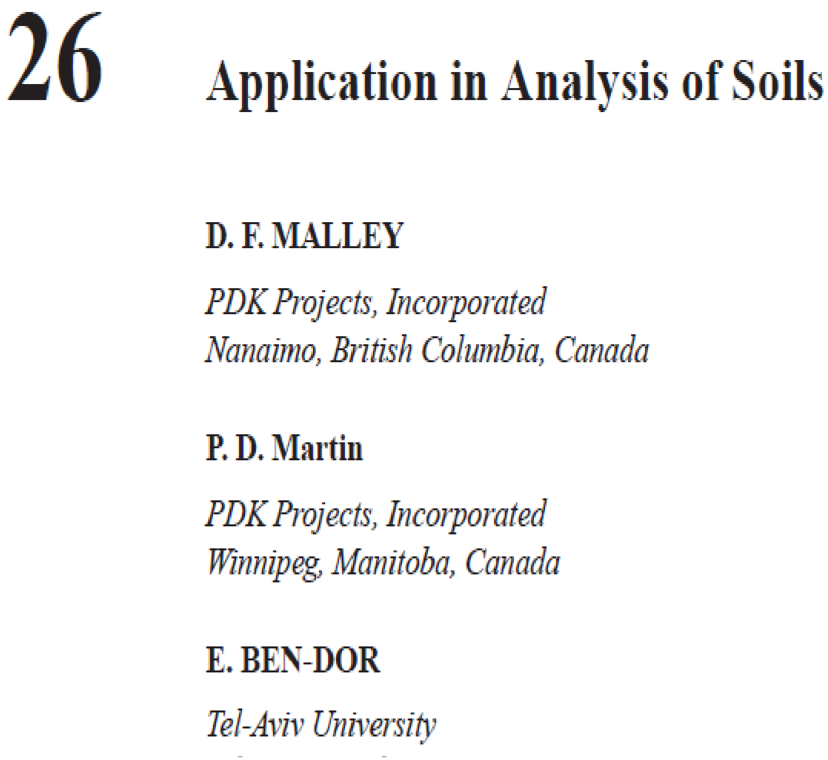
2002



26 Application in Analysis of Soils

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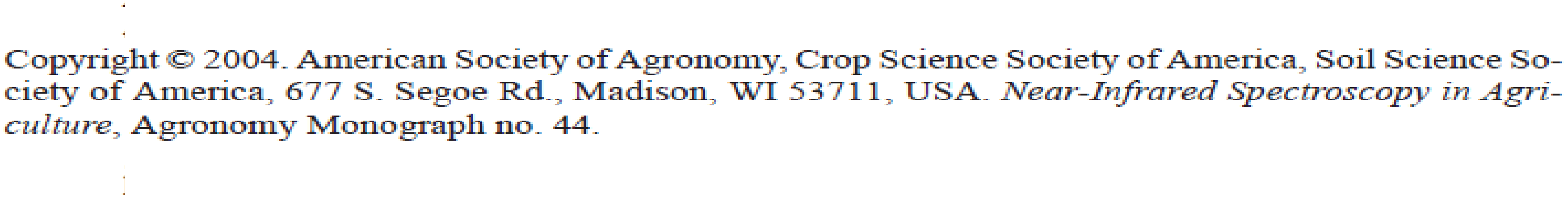
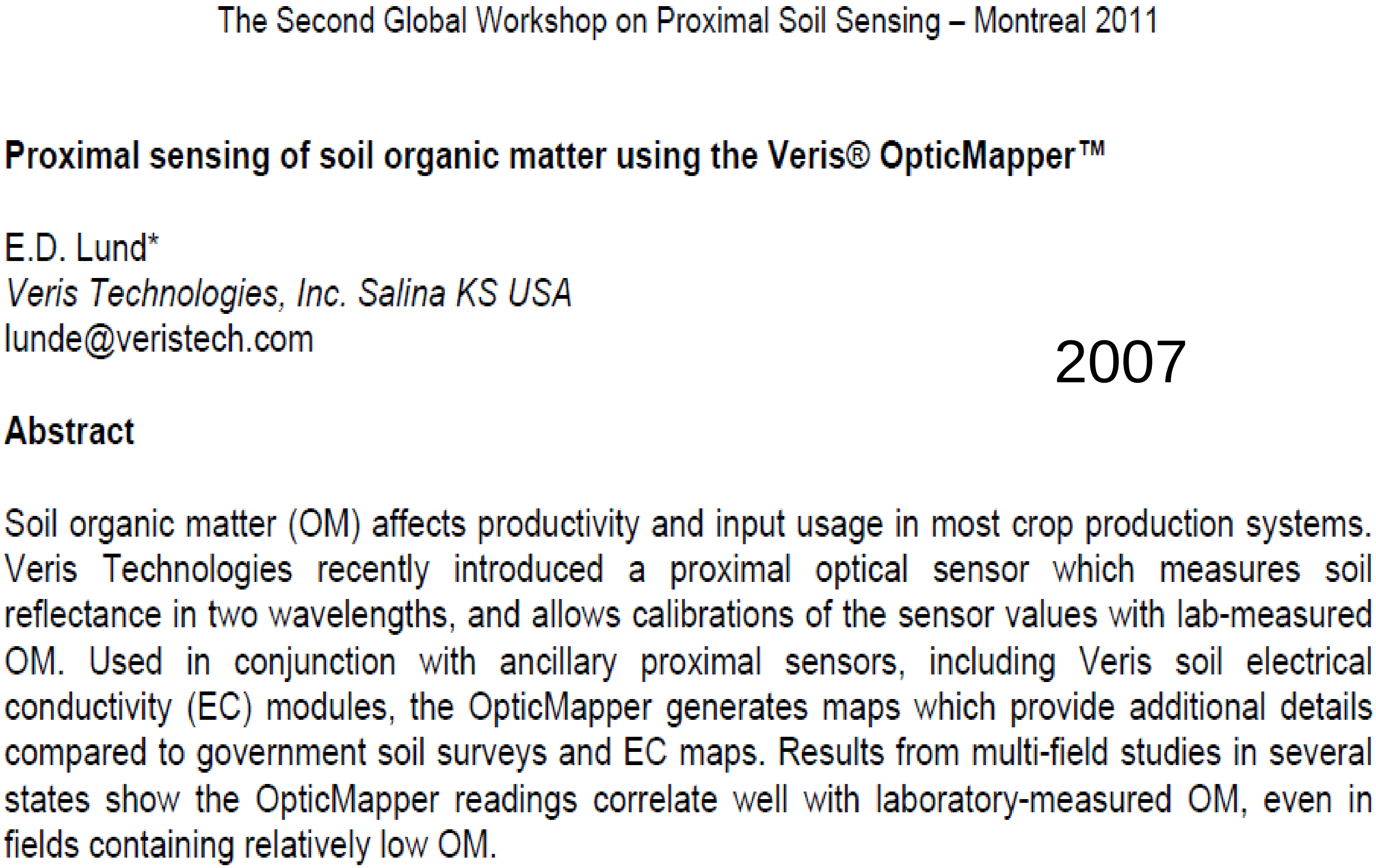


Near-Infrared Spectroscopy in Agriculture, Agronomy Monograph no. 44.

NIRS Summary

- 1968 – 1 paper (Ben Gera and Norris)
- 1986 – call to wake the giant (Davis)
- 1986 – Soil –NIRS first application (Dalal and Henry)
- 1998 - from sleeping technology to morning star (Davis)
- 2002 – NIRS – soil in HSR domain (Ben Dor et al.)
- 2004 – NIRS in Soil + other applications (Malley et al.)

- 2006 – many applications, thousands of paper, a journal (*NIRJ*), Books, fully commercialized technology



The Second Global Workshop on Proximal Soil Sensing – Montreal 2011

Proximal sensing of soil organic matter using the Veris® OpticMapper™

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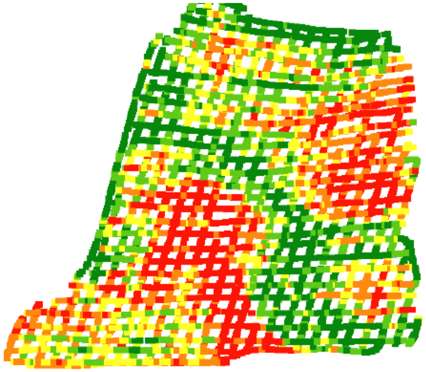
2007

Abstract

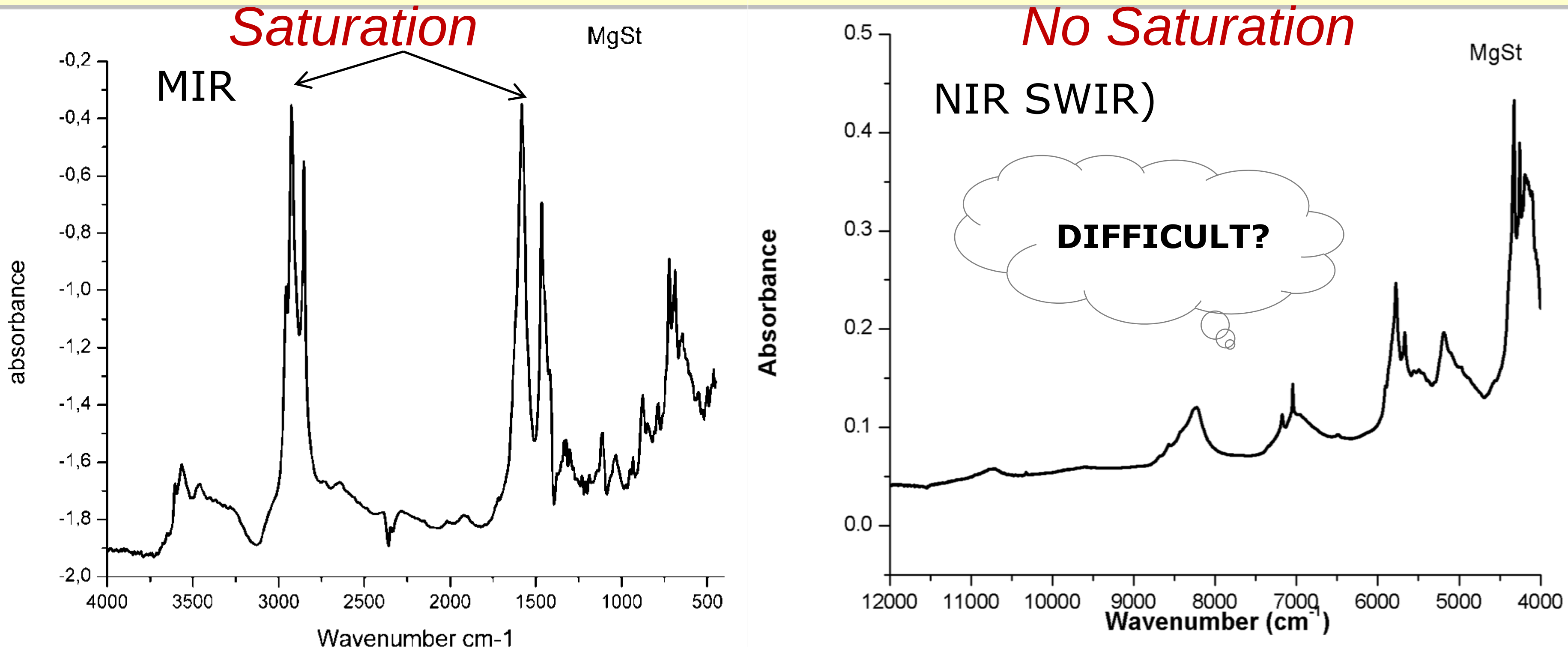
Soil organic matter (OM) affects productivity and input usage in most crop production systems. Veris Technologies recently introduced a proximal optical sensor which measures soil reflectance in two wavelengths, and allows calibrations of the sensor values with lab-measured OM. Used in conjunction with ancillary proximal sensors, including Veris soil electrical conductivity (EC) modules, the OpticMapper generates maps which provide additional details compared to government soil surveys and EC maps. Results from multi-field studies in several states show the OpticMapper readings correlate well with laboratory-measured OM, even in fields containing relatively low OM.

Industry!!!

Figure 1. Veris OpticMapper with Soil EC and Optical Sensors.



Why NIRS and not MIRS ?



Saturation

No Saturation

DIFFICULT?

MIR spectra obtained by ATR and NIR SWIR spectra obtined by Diffuse Reflectance

NIR SWIR is not saturated and hence might hold better correlcation with the atributes concentration!

Advantageous

- As spectroscopy is rapid, timely, less expensive, non-destructive, straightforward and sometimes more accurate than conventional analysis the NIRS vastly adopted by many users

- **Sample preparation is simple**
- **Waste and reagents are minimized (non-destructive testing).**
- **It can be fully automated- no skilled personal is requiered**
- **Spectral features are not satuated**
- **Low Cost**

Disadvantageous

- The development of calibrations set has to be developed for each population (to maintain the physical factors constant)

- Not as accurate as the chemical analysis

- Requires a very stable conditions (instrument, operational, illumination, geometry)

- **Near infra-red spectroscopy (NIRS) has been in routine use for the assessment of a range of components in dry materials (e.g. protein in grains).**

- **The presence of water, which also absorbs strongly in the near infra-red has limited the use of NIRS for assessment of quality of fresh produce.**

- **Water as a limited factor (governing the "real part" of the EM) used to be minimized in the first NIRS analysis.**

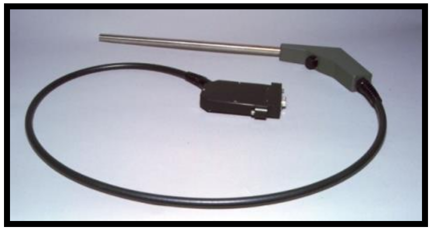
- **Recent improvements, namely, the massive increase in computing power of modern PCs and the development of software capable of carrying out the complex statistical mathematics has made the technique applicable to high moisture products such as fresh fruit.**

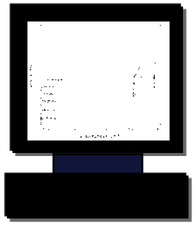
NIRS past and present

Why NIRS now?

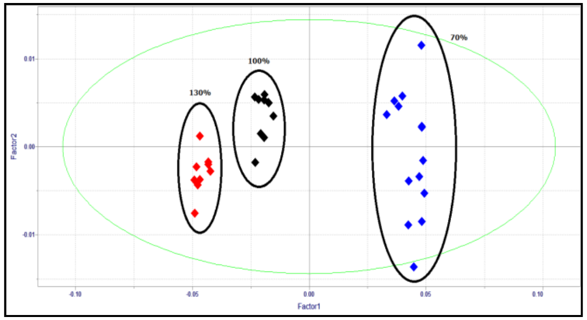
Improvements in the fields of

1. **Optical fibers + Imagina camera**

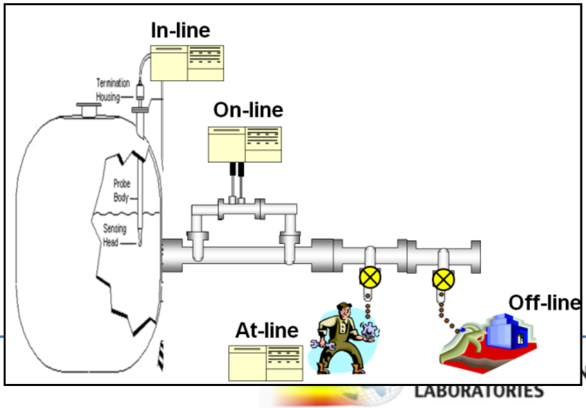




2. **Computing power**



3. **Chemometrics**

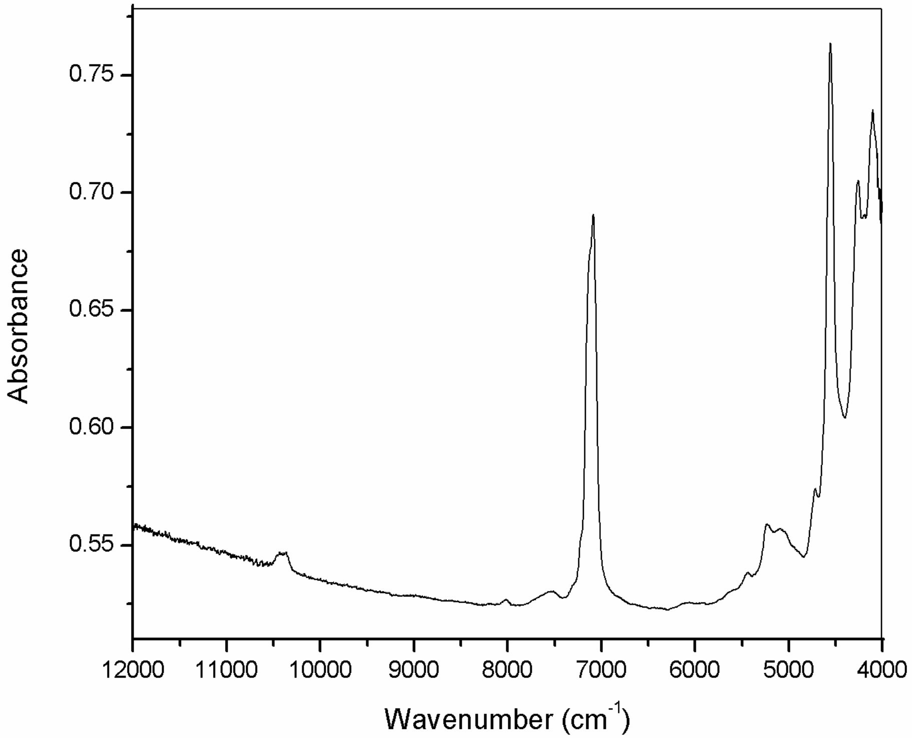


4. **Interest in procces analysis**

Advantages of NIRS

- Diagnostic tool

Lepidolite rock



Advantages of NIRS

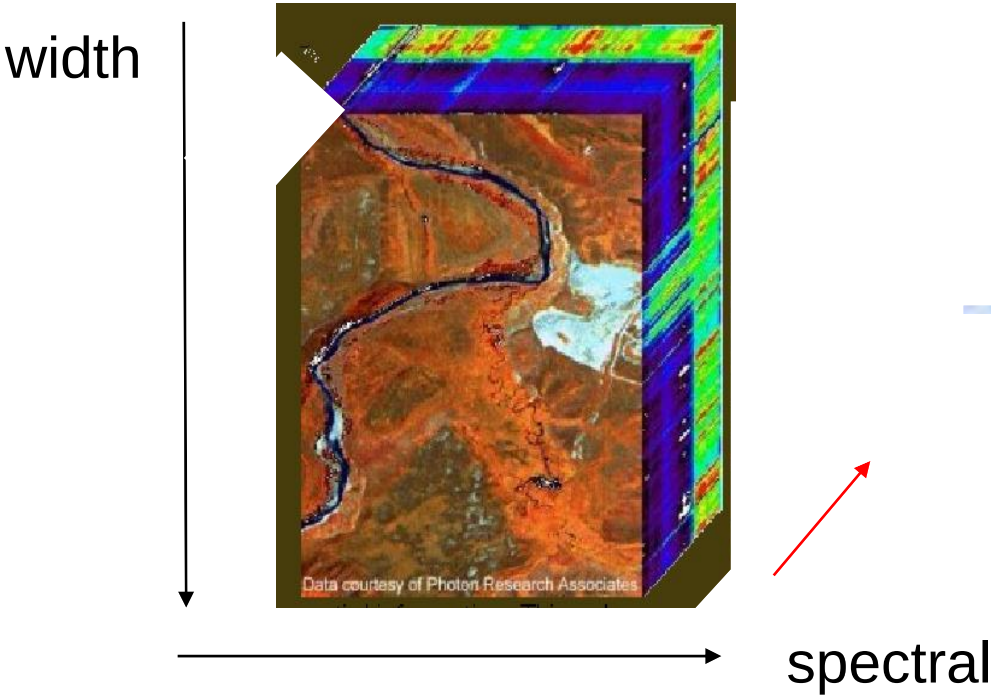
- *Spectra may be obtained in non-invasive manner.*

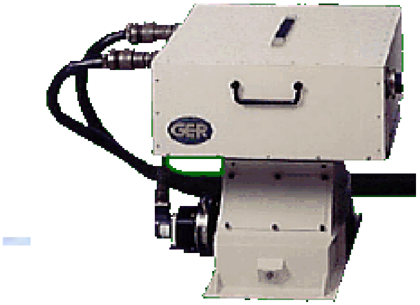
Totally non-invasive analysis of blood glucose by NIR

Advantages of NIRS

- *Remote sampling is possible (good for hazardous materials).*

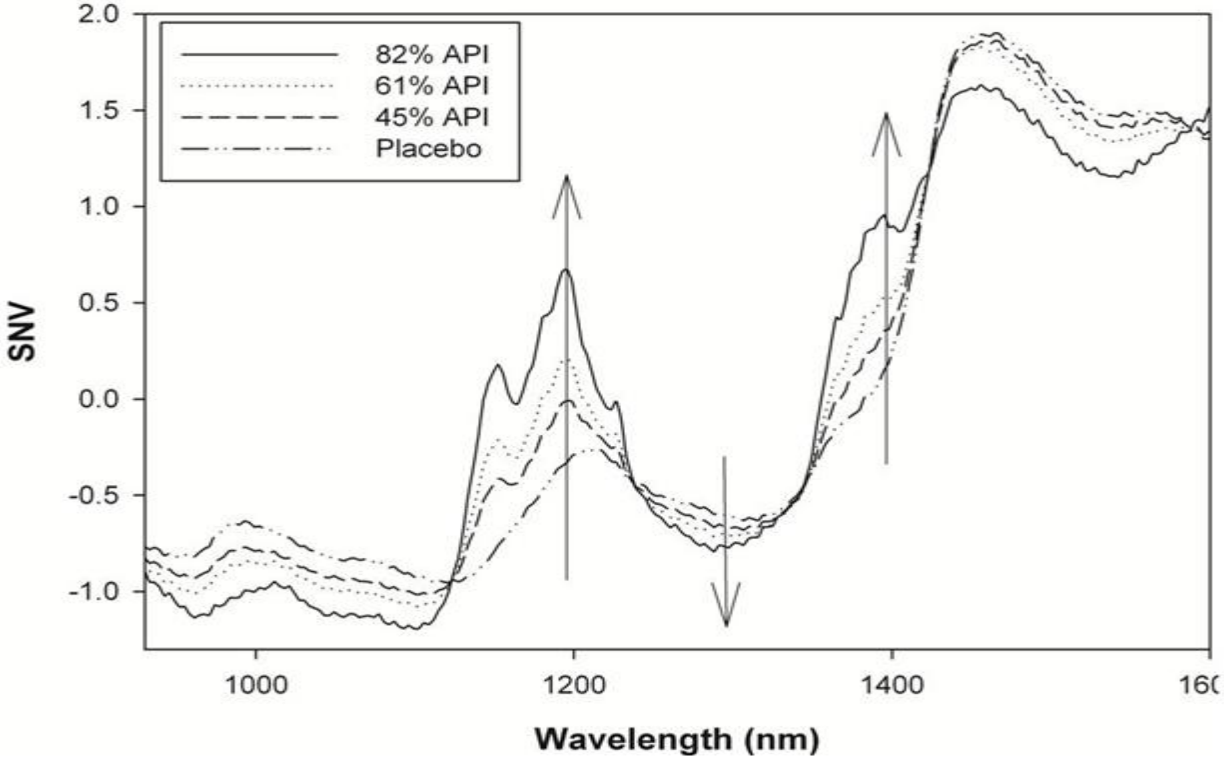
HSR: ***"The acquisition of images in hundreds of registered, contiguous spectral bands such that for each picture element it is possible to complete reflectance spectrum" (Goetz 1994)***





Advantages of NIRS

- *NIR allows us to create simple calibration models for predicting concentrations of the pharmaceutical industry in real time (during the manufacturing process)*

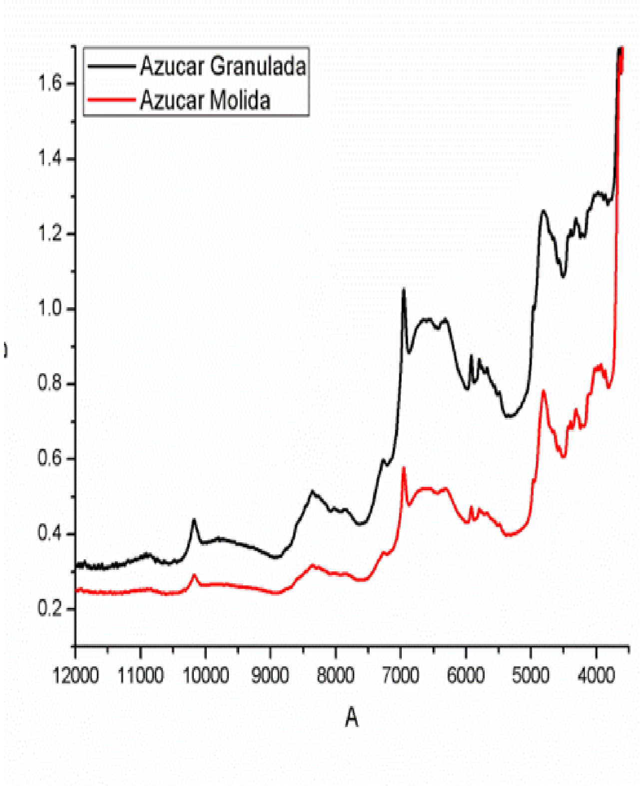


* - M. Blanco, J. Coello, A. Eustaquio, H Iturriaga, and S. Maspoch, Development and Validation of a Method for the Analysis of a Pharmaceutical Preparation by Near-Infrared Diffuse Reflectance Spectroscopy, Journal of Pharmaceutical Sciences, 1999, 88(5), 551 – 556.

Advantages of NIRS

- *Possibility of using it in a wide range of applications (physical and chemical), and viewing relationships difficult to observe by other means (**particle size distribution!**)*

Milled sugar



Granular sugar

NIRS agricultural commercial applications

- **Sorting of fruit at commercial packline speeds (melons and citrus fruit).**
- **Grains Protein Content**
- **Organic matter decomposition**
- **Soil attributes in the field**

Some Comments

- The development of a high speed system incorporated into a packing line would enable the sorting of fruit based on quality parameters such dry matter content.

- The technology may be used to exclude fruit with internal defects.

- A portable unit would enable random checks of fruit in the field, or in the wholesale or retail store.

- On-harvester estimation of grain protein content

- for precision agriculture and estimation of the sugar content of fibrated sugar cane (beet) in sugar mills.

- In the future, we should expect to see the application of NIR technology to assessing a range of food products for various aspects of quality and safety.

Commercial of Some Application

Coffee - taint analysis

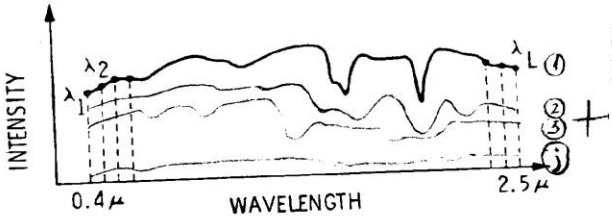
- Sweet Corn - insect damage and insect detection
- Coal - moisture determination
- Macadamia kernel - quality
- Citrus - quality attributes
- Pineapples, mango's, strawberries - quality attributes
- Stone fruit - quality attributes
- Melons - quality attributes

Quantitative Method for spectral analysis: NIRA

NIRS/NIRA is a chemomtrics method where NIR-SWIR spectral region is used to predict chemical constituents of a given matter.

b

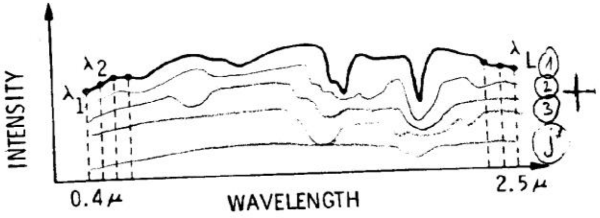
calibration



Sample Number	C1	C2 ...	Ci
1	*Cm1,1*	*Cm1,2*	*Cm1,i*
2	*Cm2,1*	*Cm2,2*	*Cm2,i*
.	.	.	.
j	*Cmj,1*	*Cmj,2*	*Cmj,i*

$\dashrightarrow$ $C_p = b_0 + b_1L_1 + b_2L_2 + b_3L_3 + \ldots + b_nL_n$

Validation



$C_p = b_0 + b_1L_1 + b_2L_2 + b_3L_3 + \ldots + b_nL_n$ $\dashrightarrow$

Concentration

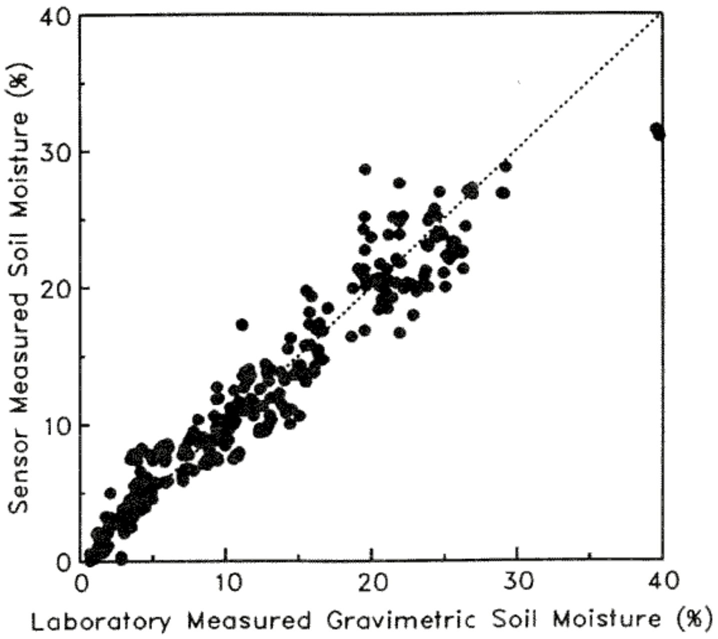
Sample Number	C1	C2 ...	Ci
1	*Cp1,1*	*Cp1,2*	*Cp1,i*
2	*Cp2,1*	*Cp2,2*	*Cp2,i*
.	.	.	.
j	*Cpj,1*	*Cpj,2*	*Cpj,i*

First developed for Food Science:

Ben-Gera, I., and K.H. Norris, 1968, Determination of moisture content in soybeans by direct spectrophotometry. Israeli Journal of Agriculture Research. 18:124-132.

Quantitative Method for spectral based SOIL properties

Dalal, R.C., and R.J. Henry. 1986. Simultaneous determination of moisture, organic carbon and total nitrogen by near infrared reflectance spectroscopy. Soil Science Society of America Journal 50:120-12



Soil- NIRS summary

- Malley D. Martin P.D. and E. Ben-Dor., 2004, Application in Analysis of Soils. Chapter 26 In *Near Infrared Spectroscopy in Agriculture.* Craig R., Windham R., and Workman J., (eds). A three Societies Monograph (ASA, SSSA, CSSA) 44: 729-784.

- Viscarra Rossel R.A., D.J.J Walvoort, A.B. McBratney, L.J. Janik and J.O. Skjemstad 2006 Visible, near infrared, mid infrared or combined diffuse reflectance spectroscopy for simultaneous assessment of various soil properties *Geoderma* 131:59-75.

- Demattê, J.A.M., Campos, R. C., Alves, M. C., Fiorio, P. R. and Nanni, M. R. 2004c. Visible-NIR reflectance: a new approach on soil evaluation. *Geoderma*, 121: 95-112.

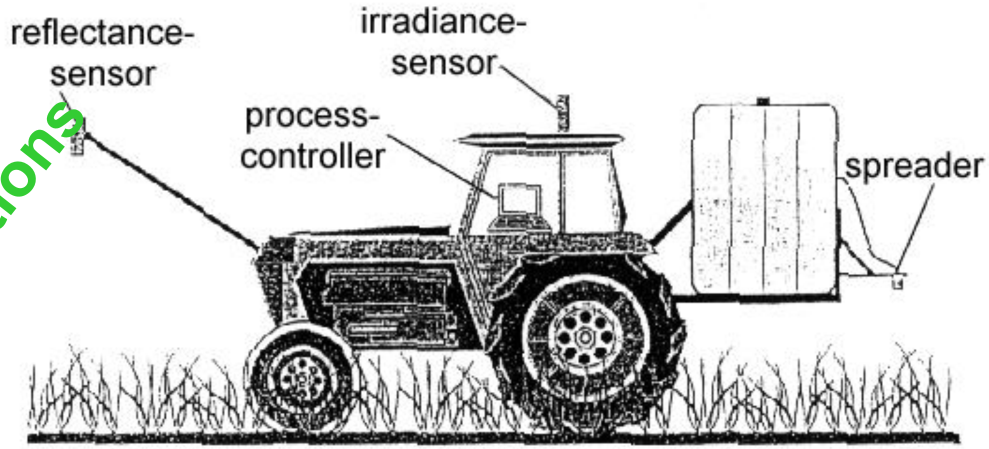
Conclusions

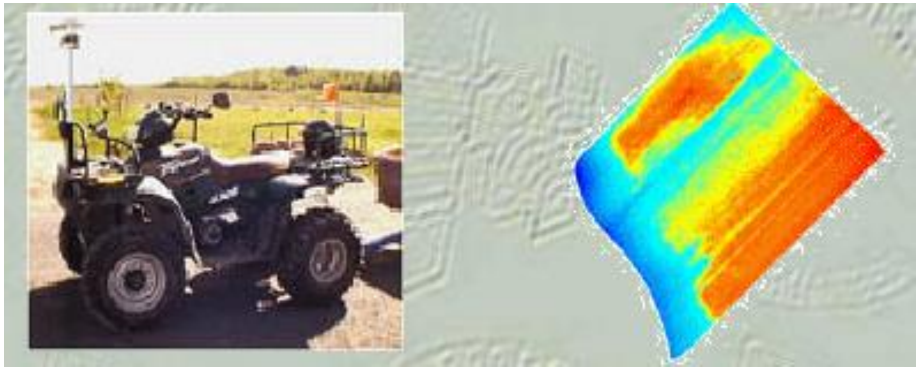
- Soil is a complex system
- Soil Spectra consists of many interesting chromophores
- Quantitative analysis of soil spectra is possible (NIRS)

Idea: to apply NIRS or related methods to precision agriculture domain (1999)

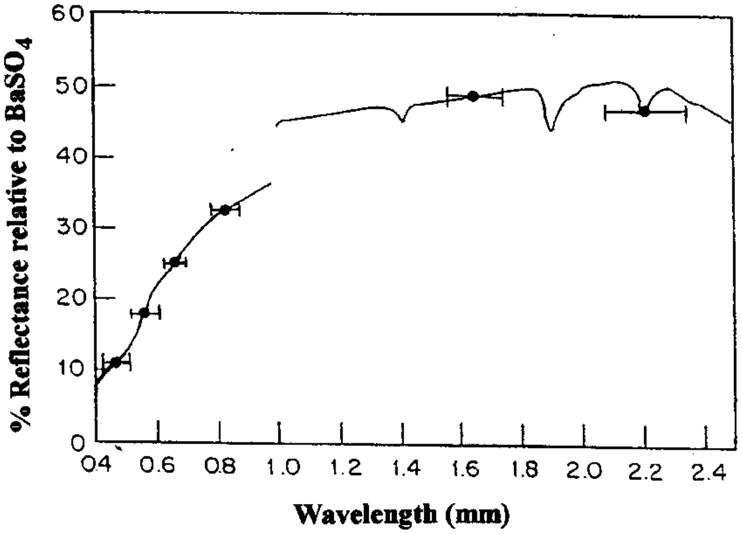
2013- ready

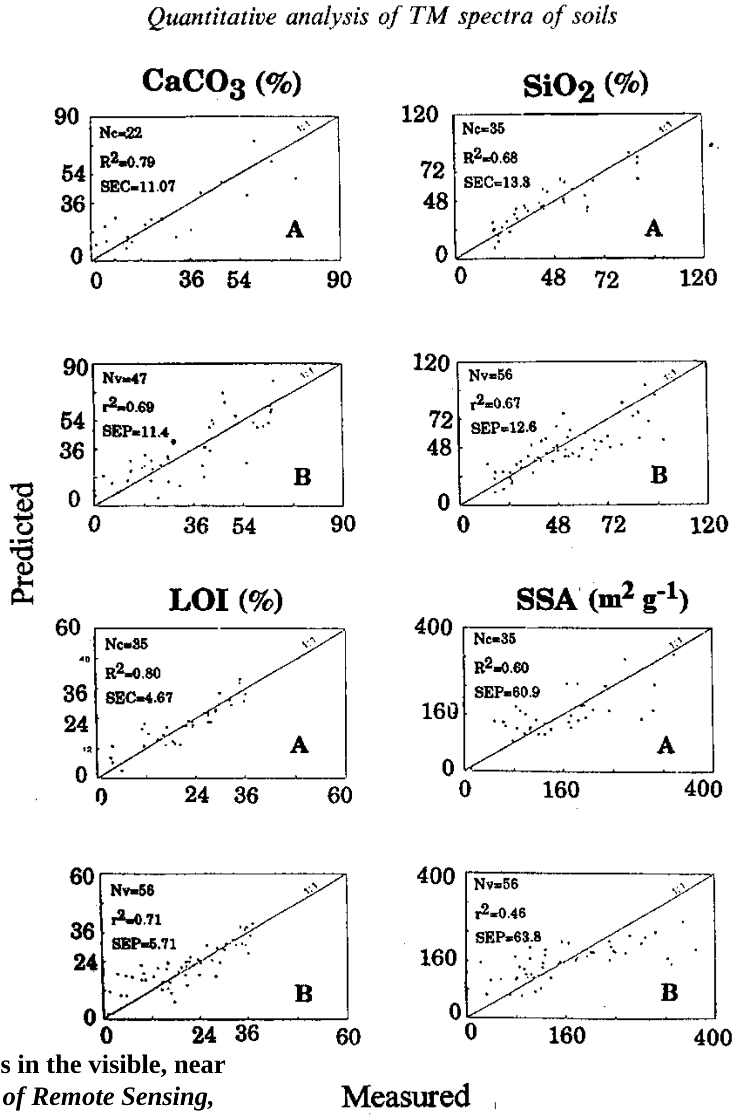
Ideas rather applications





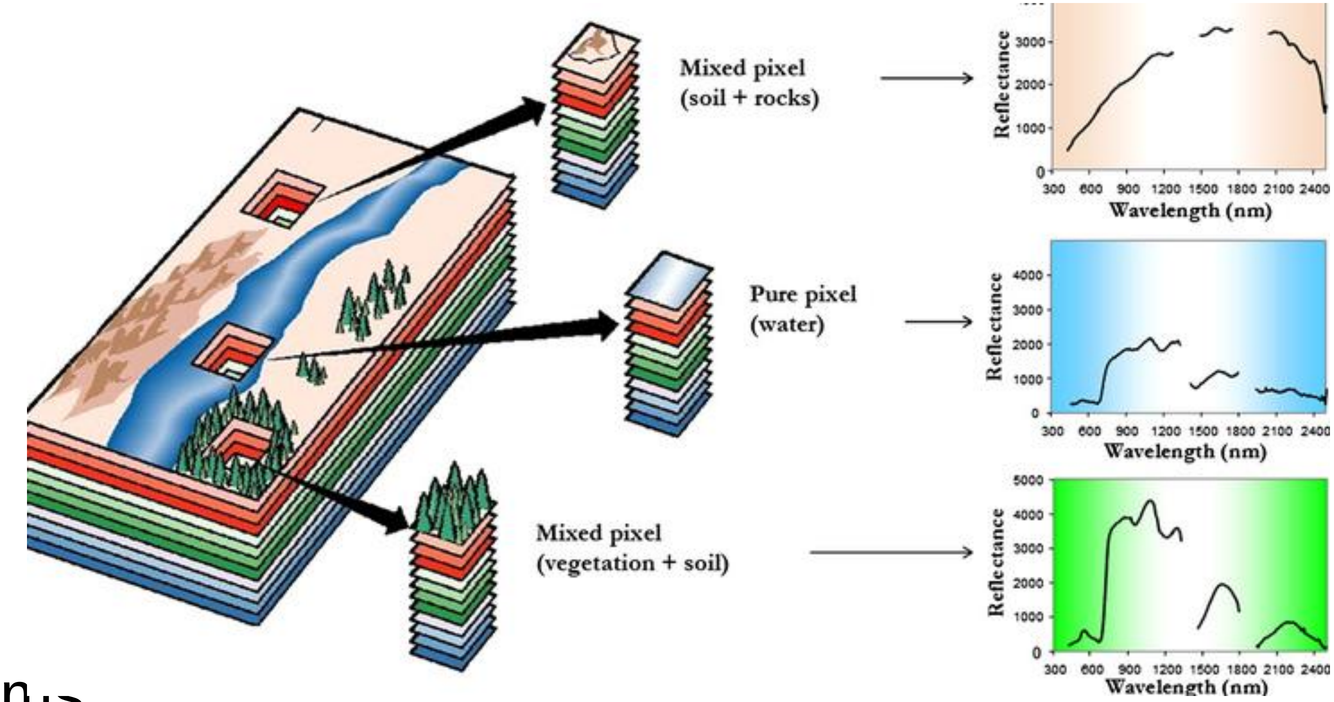
NIRS can be run in 6 TM bands





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.**

Applying ***Hyperspectral Remote Sensing (HSR)***

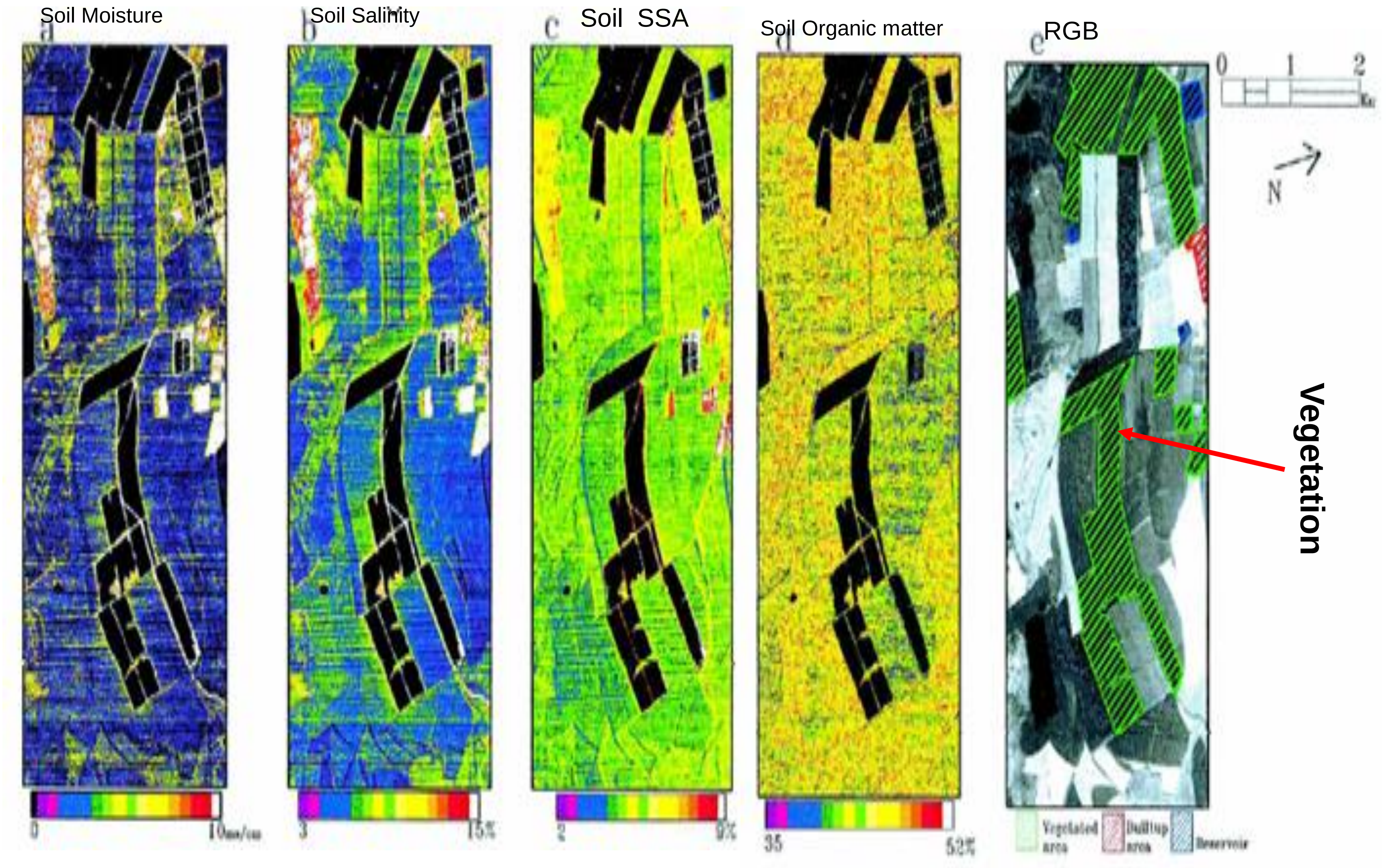


Problems

- Atmosphere,
- Instrument
- Surface

NIRS can be used in HSR domains

Ben-Dor et al., 2004


Soil Moisture

Soil Salinity

Soil SSA

Soil Organic matter

RGB

Vegetation

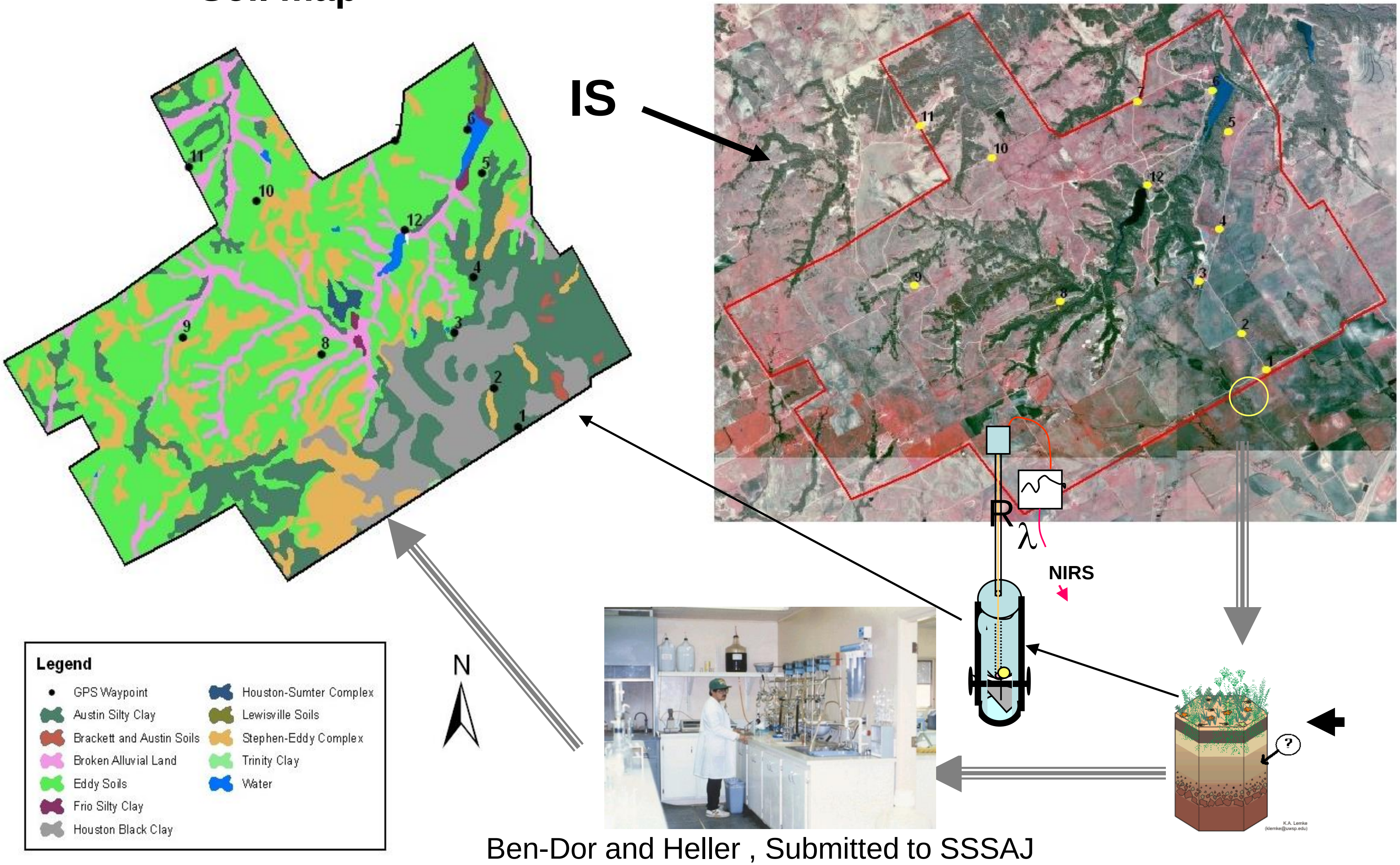
Quantitative IS of soil properties

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

Soil map production

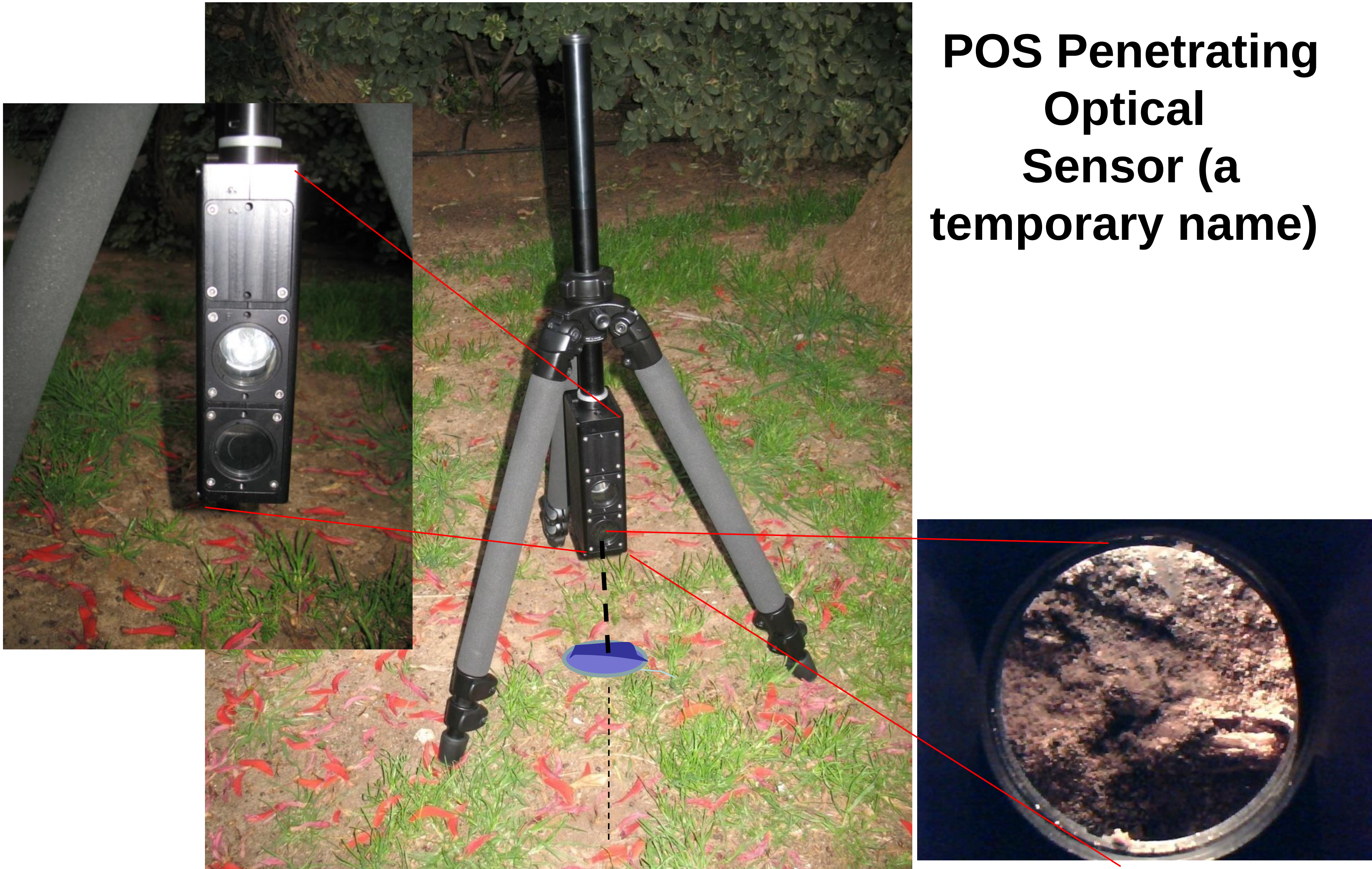
Soil map

Air photograph

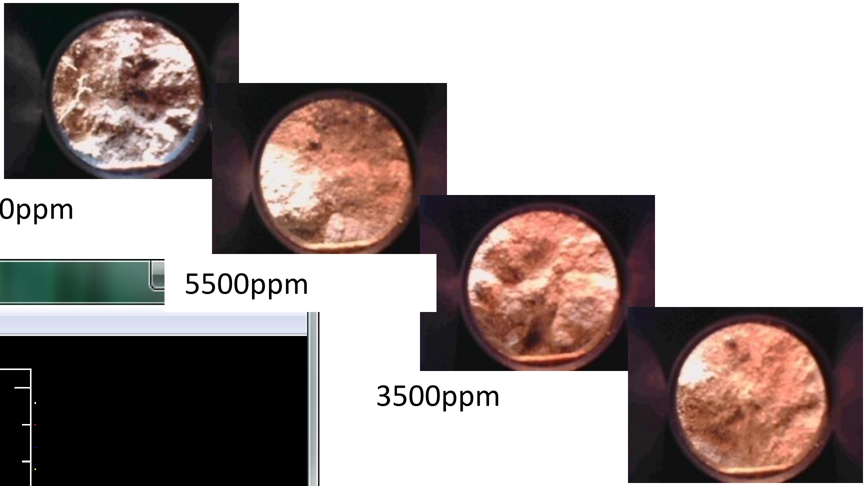


Ben-Dor and Heller , Submitted to SSSAJ

POS Penetrating Optical Sensor (a temporary name)



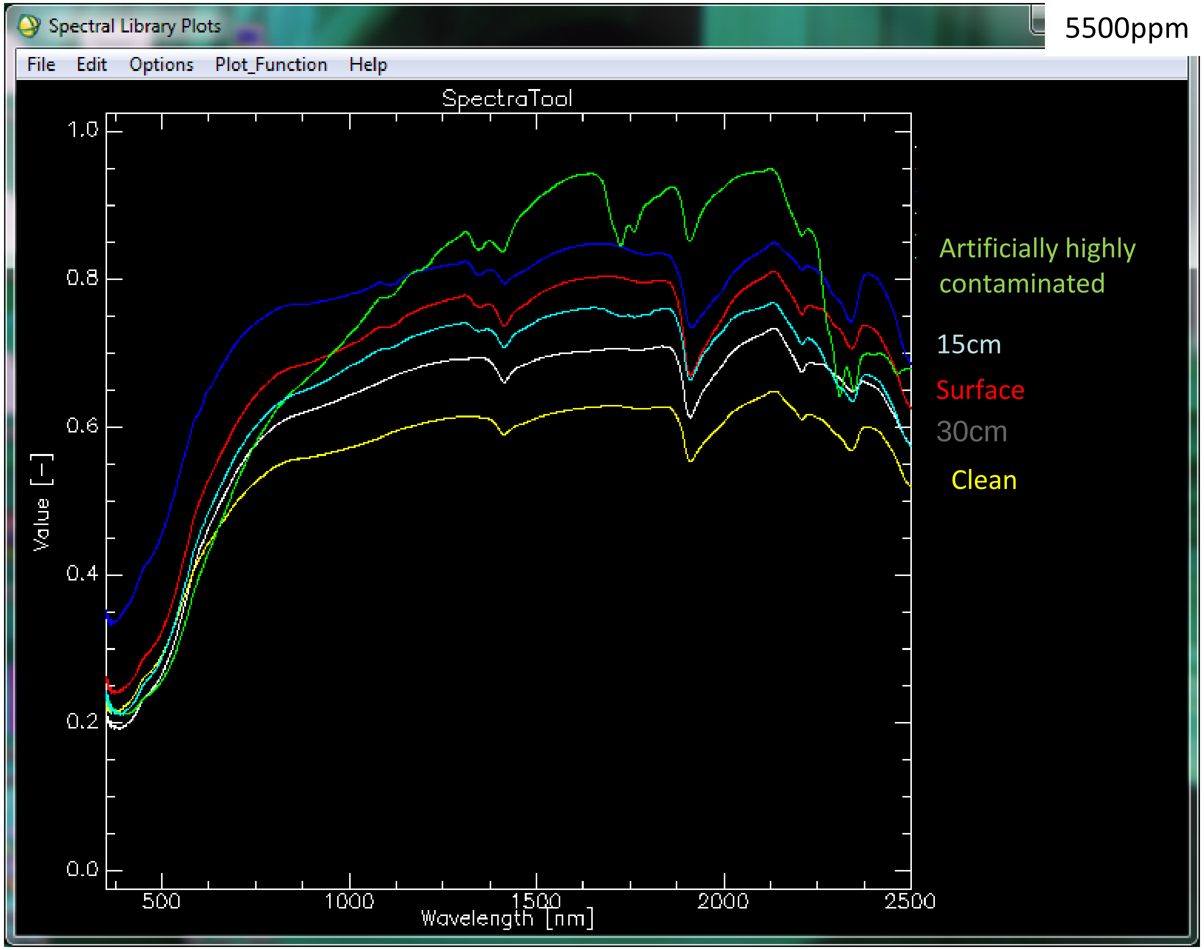
Penetrating soil profile measurements

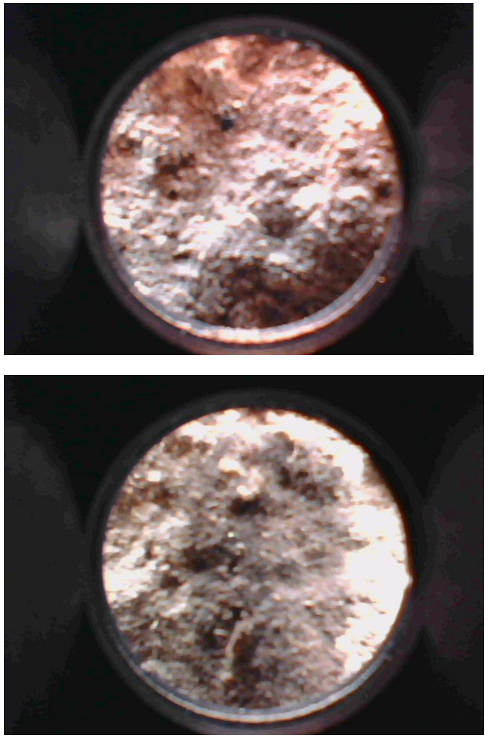


1500ppm

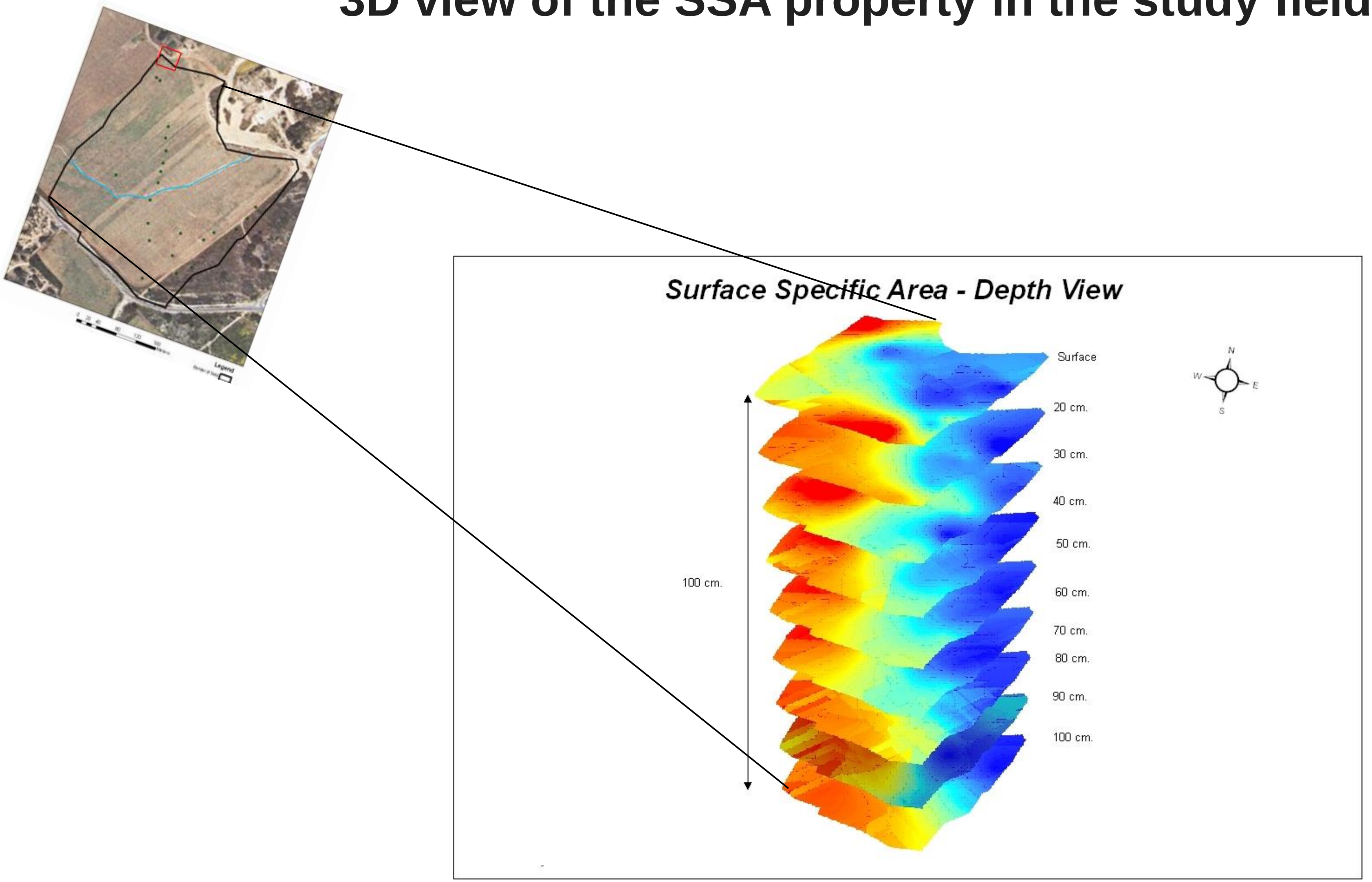
5500ppm

3500ppm

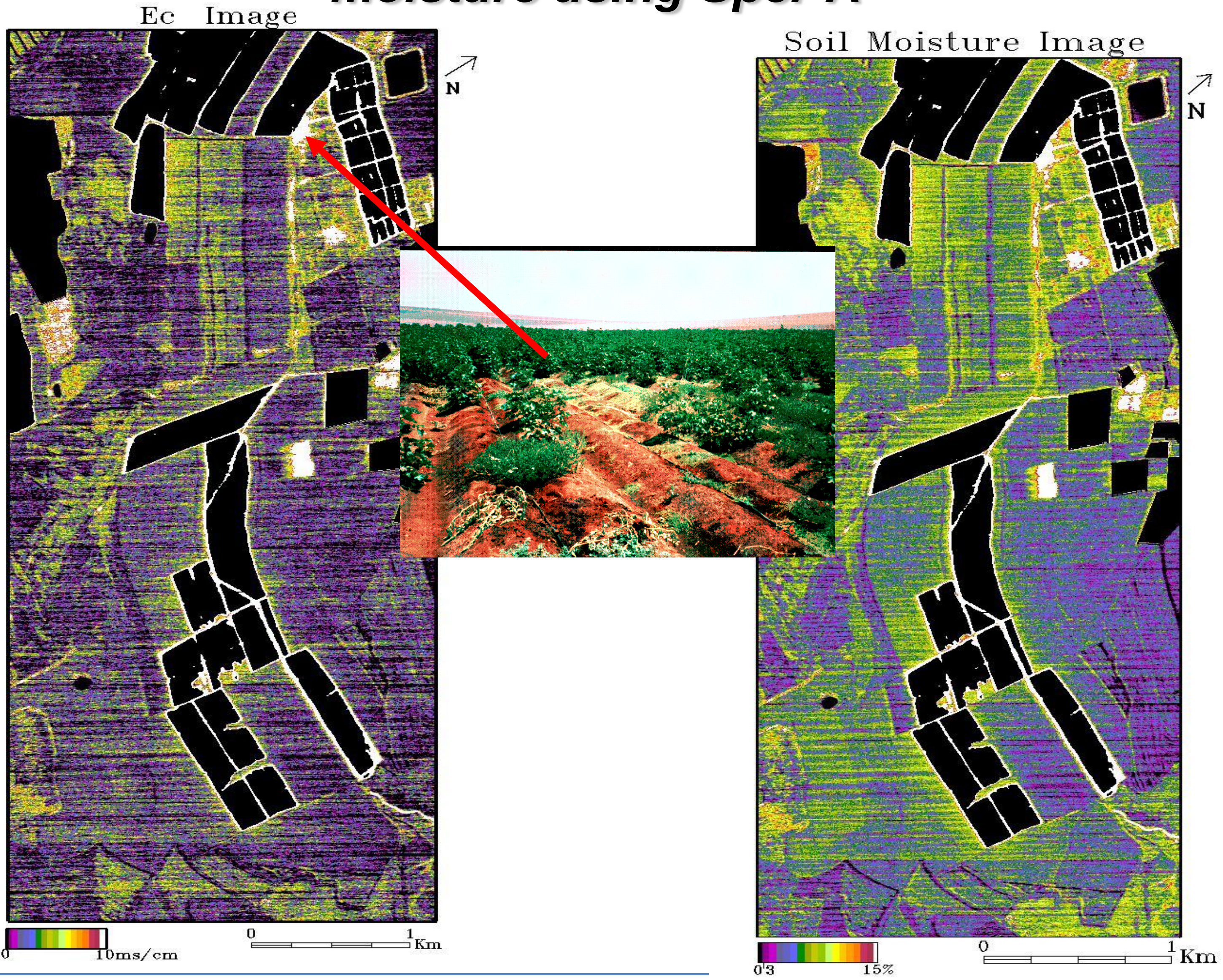




3D view of the SSA property in the study field

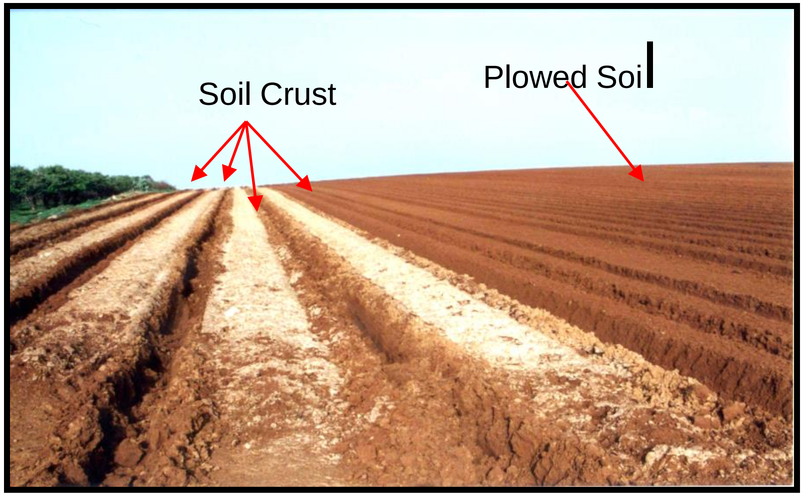


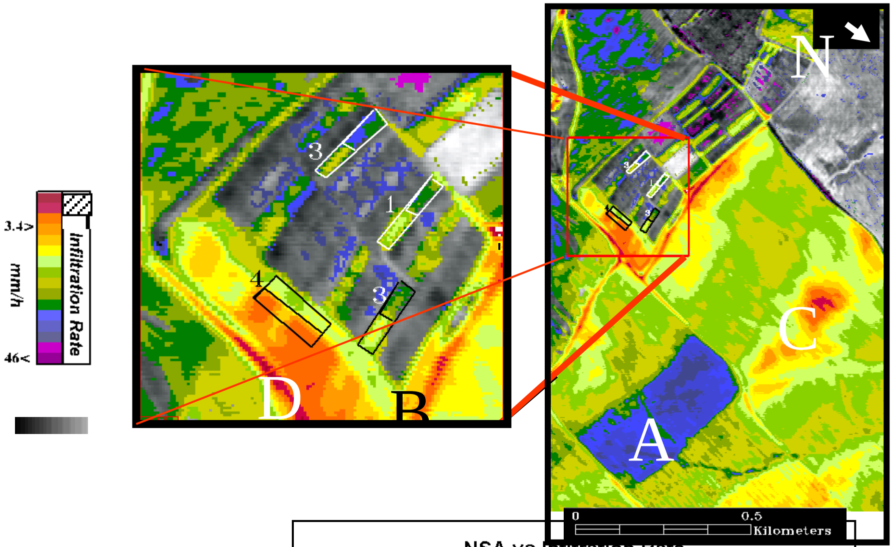
Hyperspectral sensong of soil salinity and moisture using Sper-A

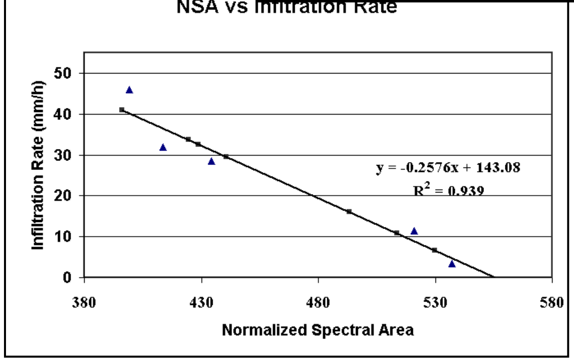


Ben-Dor E., K. Patkin, A. Banin and A . Karnieli 2002 Mapping of several soil properties using DAIS-7915 hyperspectral scanner data. A case study over clayey soils in Israel. *International Journal of Remote Sensing* 23:1043-1062

Physical Crust







0 joule

650 joule

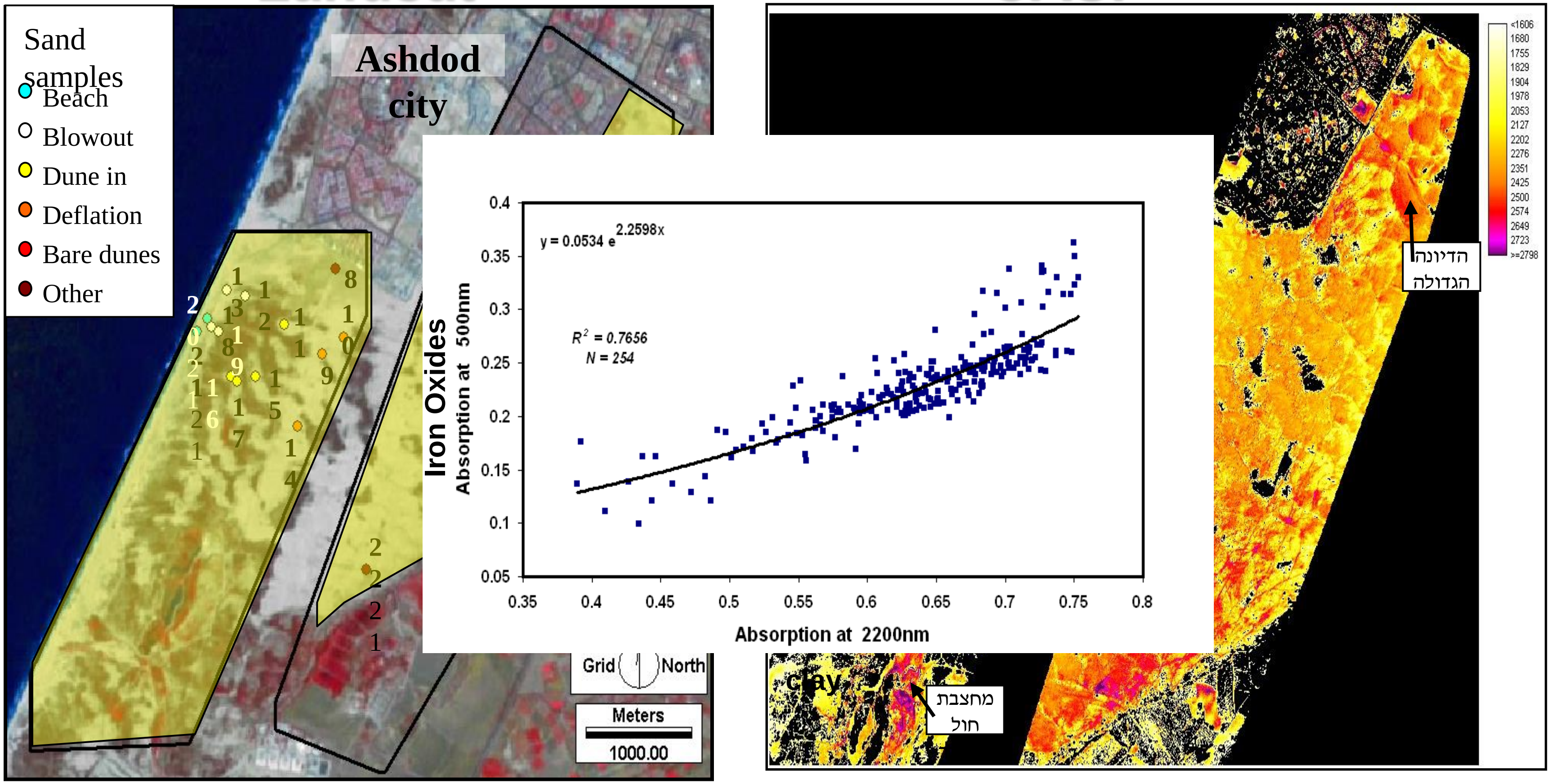
1842 joule

Ben-Dor E. , N. Goldshalager, O. Braun , B. Kindel , A.F.H.Goetz , D. Bonfil , M. Agassi, N. Margalit , Y. Binayminy and A. Karnieli *2004* Monitoring of Infiltration Rate in Semiarid Soils using Airborne Hyperspectral Technology *International Journal of Remote Sensing* 25:1-18

Soil Formation

Ben-Dor et al., 2005

Landsat **CASI**

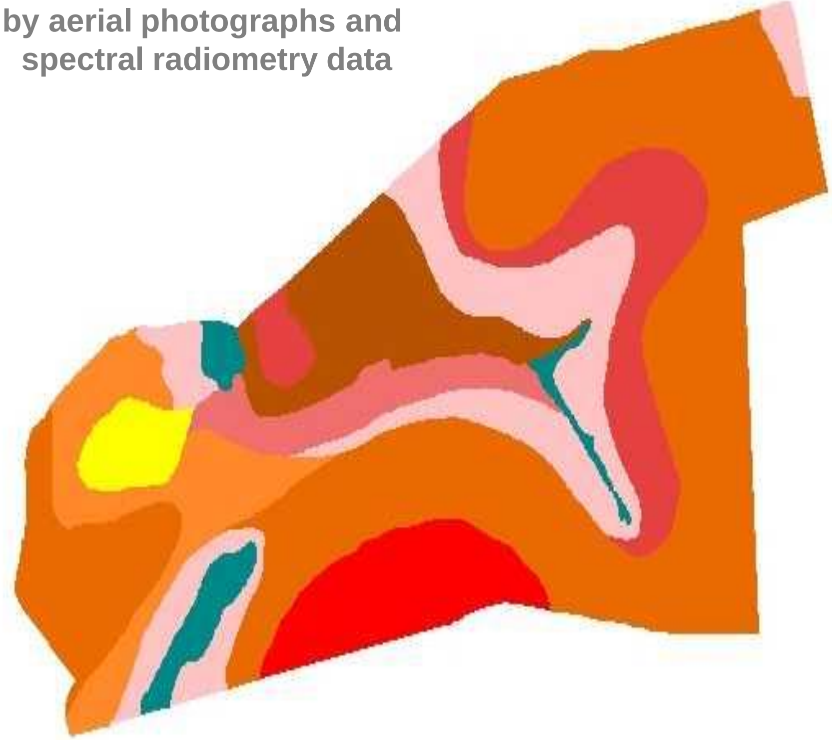


Iron oxides as indicator for soil formation

Soil mapping from field spectroscopy

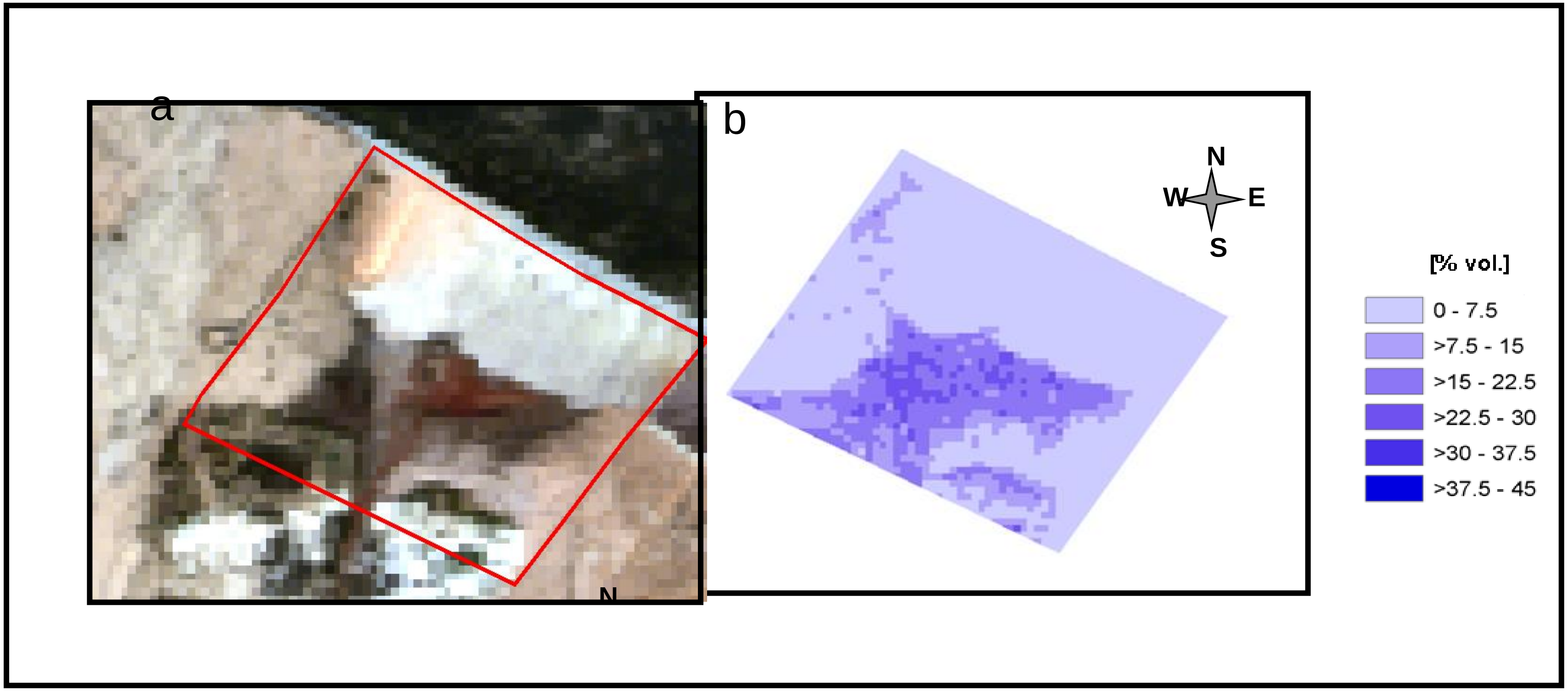
Detailed soil map constructed
by traditional methods

Detailed soil map constructed
by aerial photographs and
spectral radiometry data



Soil Water content

Haubrock et al., 2006b



Problems with HSR of soils

- Heterogeneity due to the large pixel size
- Atmosphere attenuations
- Signal to noise of air born sensor are lower than field and lab sensors
- All models are available for mixed soil and 2mm< grain size
- Crust may mask the real A0
- Dust may mask the real A0
- Reputability of soil spectra in the field of not yet known