Utilization of the Internal Soil Standard (ISS) Method to Optimize the Exchange of Soil Spectral Libraries

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3- Czech Geology Survey, Czech Republic
4- University of Sao Paulo

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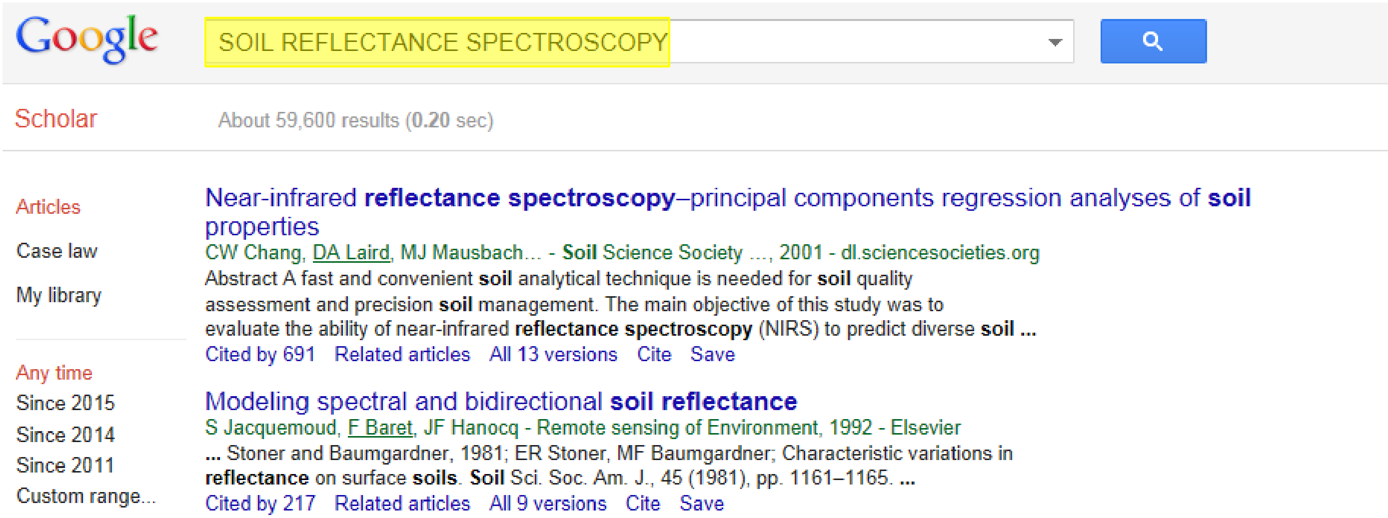
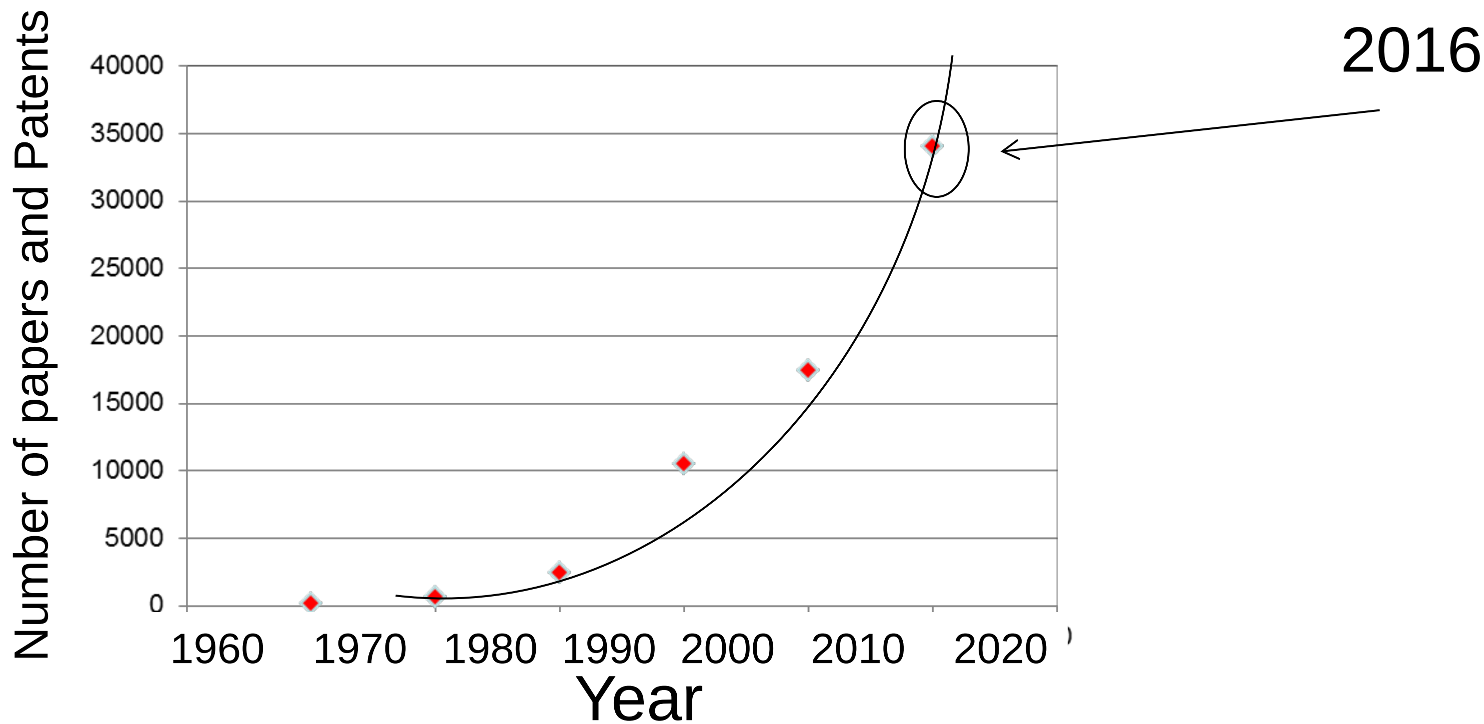
Outline

1) Soil Spectroscopy : The Importance
2) Soil Spectral Library: The Importance for DSM
3) Soil Spectroscopy : The problem and suggested solution
4) Internal Soil Standard (ISS): The idea
5) First Results: *Prones and Cones*
6) Further Development: ideal internal samples
7) Validation Results: Different protocols, laboratories & sensor
8) Conclusions

The Importance of Soil Spectroscopy





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The Importance of Soil Spectral Library:

(The World Spectral Group data base, Viscarra Rossel 2015)

The data based is composed of:

1)About 23,631 Soil Spectra

2)About 5 Soil Attributes

A global spectral library to characterize the world's soil

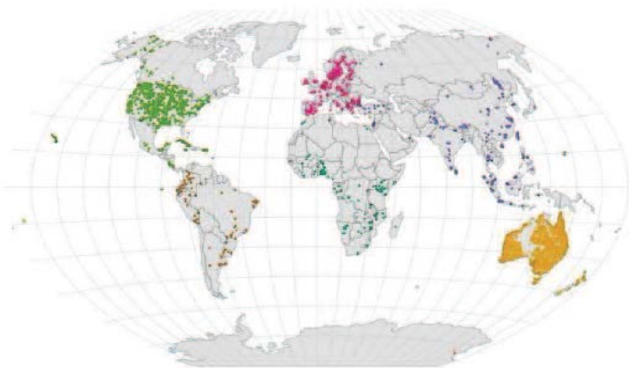
ARTICLE in EARTH-SCIENCE REVIEWS · FEBRUARY 2016
Impact Factor: 7.89 · DOI: 10.1016/j.earscirev.2016.01.012

The measurement were acquired by:

1)60 Instruments

2) >80 users

3) around 40 Protocols



The soil attributes were evaluated by:

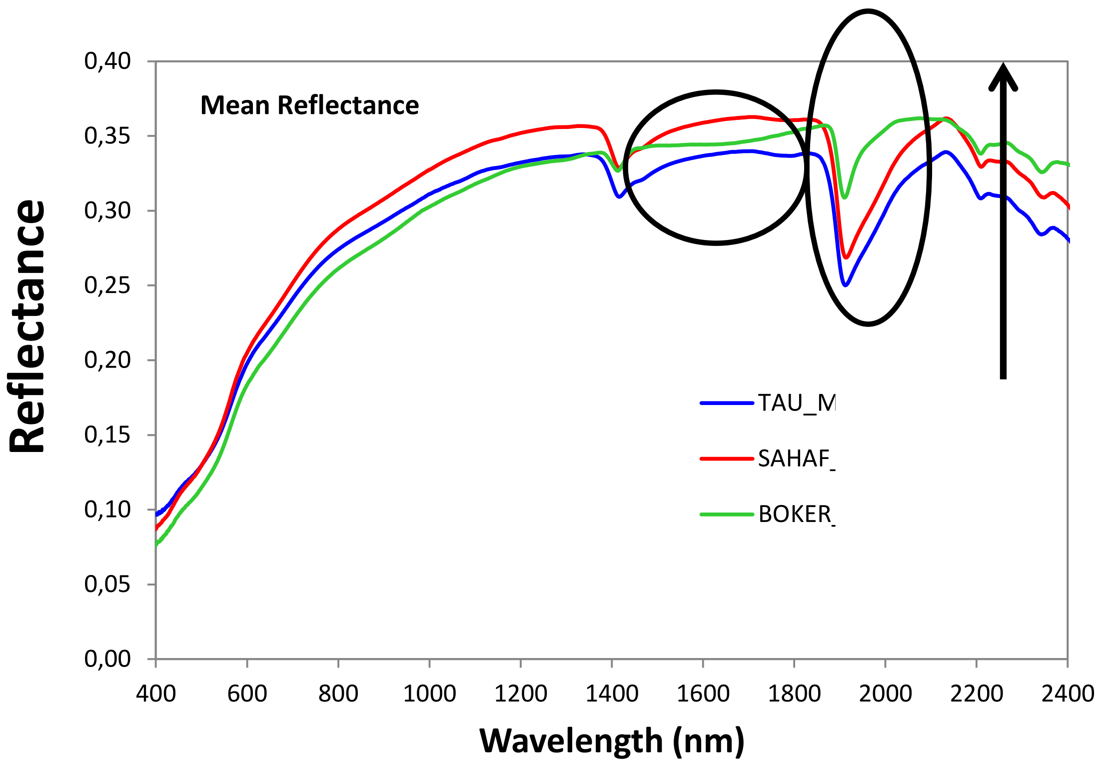
1) Standard methods (e.g. Jackson 1966)

R.A. Viscarra Rossel, T. Behrens, E. Ben-Dor, D.J. Brown, J.A.M. Demattê, K.D. Shepherd, Z. Shi, B. Stenberg, A. Stevens, V. Adamchuk, H. Aïchi, B.G. Barthès, H.M. Bartholomeus, A.D. Bayer, M. Bernoux, K. Böttcher, L. Brodský, C.W. Du, A. Chappell, Y. Fouad, V. Genot, C. Gomez, S. Grunwald, A. Gubler, C. Guerrero, C.B. Hedley, M. Knadel, H.J.M. Morrás, M. Nocita, L. Ramirez-Lopez, P. Roudier, E.M. Rufasto Campos, P. Sanborn, V.M. Sellitto, K.A. Sudduth, B.G. Rawlins, C. Walter, L.A. Winowiecki, S.Y. Hong, W. Ji

http://groups.google.com/group/soil-spectroscopy/files

The Problems - Example 1: *Spectral Domain*

One soil: Three different protocols



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The problem - Example 2: *Analytical Domain*

100 samples (60 cal, 40 val) – three protocols : Quantitative analysis

Instrument / Operator	Internal standard	$CaCO_3$	Clay Content	Organic Matter	Fe2O3
		RMSEP	RMSEP	RMSEP	RMSEP
TAU	**Original**	**13.24**	**5.4**	**1.54**	**4316**
SAHAF	Original	13.33	8.2	1.50	5169
BOKER	Original	17.44	8.9	1.79	4687

The internal standard idea was adopted from the **analytical chemistry** discipline

Internal Standard Method Calculations

Auswertung mit Hilfe des inneren Standards

Calculs employés dans la methode de dosage avec étalon interne

D. E. Willis

Research Specialist, Monsanto Company, 800 N. Lindbergh Boulevard, St. Louis, Missouri 63166, USA

$$F_R(i) = (\text{counts/gram})_{\text{standard}} / (\text{counts/gram})_{\text{component } i} \quad (1)$$

Quantitation of samples containing non-volatile components (e. g. resins or tars) or components to which the detector is insensitive (e. g. fixed gases or water with flame ionization detector) is a problem continually facing many chemists using gas chromatographic methods. Two methods can be used to solve this problem:

a) calibration on an absolute basis by injection of the same amount of sample for each analysis, or
b) use of the internal standard method.

The first method involves the preparation of standards bracketing the range in which the component(s) of interest will lie and requires considerable skill to precisely inject the same weight of sample each time. Application of this method to multicomponent mixtures can hardly be re-

The internal standard method involves the addition of a known amount of a pure substance to a known weight of sample. The requirements for a substance used as an internal standard are:

a) must yield a completely resolved peak,
b) should elute close to the component(s) being measured,
c) should not be present in the original sample,
d) must not react chemically with the sample, and
e) should be present in about same concentration as components measured.

Requirement (a) is to insure a unique and unambiguous area for the peak; (b) is to minimize any change in detector response due to changes in operating conditions (flow, temperature, etc.); (c) and (d) insure tl : of

Pimstein's paper

SSSAJ: Volume 75: Number 2 • March–April 2011 1

A first attempt to demonstrate the Internal Standard idea for soil spectroscopy

Important conclusions for using Internal standards for soil

Soil Mineralogy

Performance of Three Identical Spectrometers in Retrieving Soil Reflectance under Laboratory Conditions

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A wide range of electronic and mechanical noise factors can affect soil spectra when using different instruments or even when repeating a specific sample's measurements with the same spectrometer. In soil samples where very weak spectral features are monitored for chemometric purposes, alterations in wavelength location, peak absorption shape, or albedo intensity can limit the use of previously developed spectral models. To quantify this alteration and propose a standardization method, 12 soil samples and three different materials for internal standards (sand, glass and polyethylene) were analyzed. This population was concurrently measured with three identical spectrometers using a strict measurement protocol, and then by different operators with different protocols. Significant changes in the soil spectra were found when different operators performed the measurements, being reduced >50% when the strict protocol was applied. Sand was found to be the ideal internal standard for correcting the spectra to a reference spectrometer, even when different measuring protocols were used. This standardization also showed an improvement in the prediction of soil properties when applying chemometric spectral models even with different instruments, concluding that the use of an internal standard and a strict protocol must be applied for soil spectral measurements. As the measuring factors described in this research also affect any infrared diffuse reflectance spectroscopy measurements, the proposed method should be applicable to any instrumentation and configuration being used. This is crucial to enabling spectral comparisons between different spectrometers or, more importantly, to establishing robust chemometric models and to exchange soil spectral information.

Abbreviations: ASD, Analytical Spectral Devices, Inc.; CR, continuum removal; NIRS, near infrared analysis; PLS, partial least squares; RGB, red-green-blue color model; RMSEP, root mean square error of prediction; SAM, spectral angle mapper; TAU, Tel Aviv University.

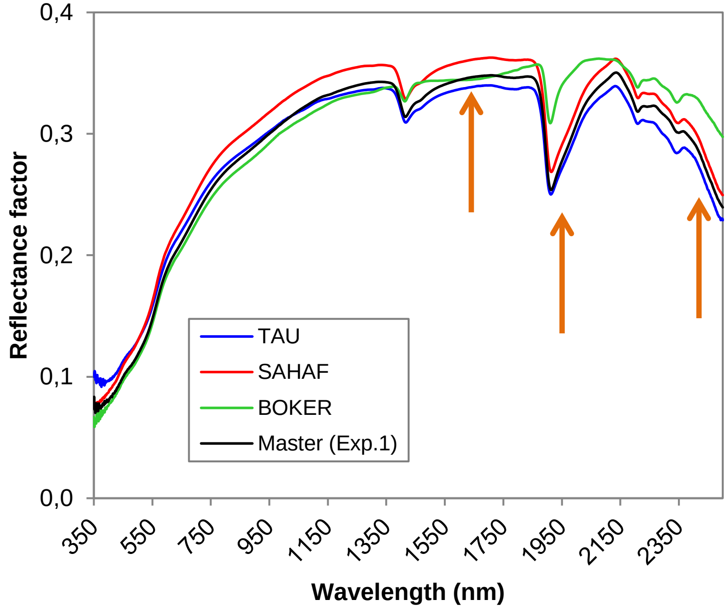
Many reflectance spectroscopy applications have been developed for soils in the last 20 yr (Malley et al., 2004). Today, reflectance in the VIS-NIR-SWIR region is considered to be a solid and mature technique for qualitative and quantitative

- 3 ASD,
- 3 Laboratories and
- 3 Climate environment
- 3 Users

Results - Standardization

Soil B spectrum comparison before and after *Sand* standardization

Original



$$CF_{\lambda} = 1 - ((S\rho_{\lambda} - M\rho_{\lambda}) / S\rho_{\lambda})$$

$$Rc_{\lambda} = Ro_{\lambda} \times CF_{\lambda}$$

$S\rho_{\lambda}$ is the reflectance of the *Slave* reference (*your measurement of the ISS)*

$M\rho_{\lambda}$ is the reflectance of the *Master* reference (*standard ISS measured by a certified agreed-lab*)

Rc_{λ} is the corrected sample reflectance (to the internal standard conditions, *standard*)

Ro_{λ} is the original sample reflectance (*sample*)

Soil NIRS

Partial Least Squares Regressions

Instrument / Operator	Internal standard	$CaCO_3$		Clay Content		Organic Matter		FeOs	
		RMSEP	Dev. (%)	RMSEP	Dev. (%)	RMSEP	Dev. (%)	RMSEP	Dev. (%)
TAU	Original	13.24		5.4		1.54		4316	
SAHAF	Original	13.33		8.2		1.50		5169	
BOKER	Original	17.44		8.9		1.79		4687	
TAU	*Formica*	13.33	0.7	5.2	-4.5	1.58	2.3	4546	5.3
SAHAF	*Formica*	16.49	23.8	8.2	0.1	1.71	13.9	4873	-5.7
BOKER	*Formica*	13.88	-20.4	5.8	-35.2	1.58	-11.8	4013	-14.4
TAU	*Sand*	**13.35**	**0.8**	**5.1**	**-5.8**	**1.55**	**0.2**	**4276**	**-0.9**
SAHAF	*Sand*	**13.27**	**-0.4**	**6.0**	**-26.7**	**1.49**	**-0.3**	**4265**	**-17.5**
BOKER	*Sand*	**13.41**	**-23.1**	**5.2**	**-42.2**	**1.56**	**-12.7**	**3927**	**-16.2**
TAU	*Glass*	15.21	14.9	9.4	74.4	1.77	14.6	6002	39.1
SAHAF	*Glass*	14.99	12.5	4.7	-42.4	1.63	8.6	4387	-15.1
BOKER	*Glass*	13.47	-22.8	6.1	-32.4	1.60	-10.4	4280	-8.7

Pimestein's Conclusion (1) :

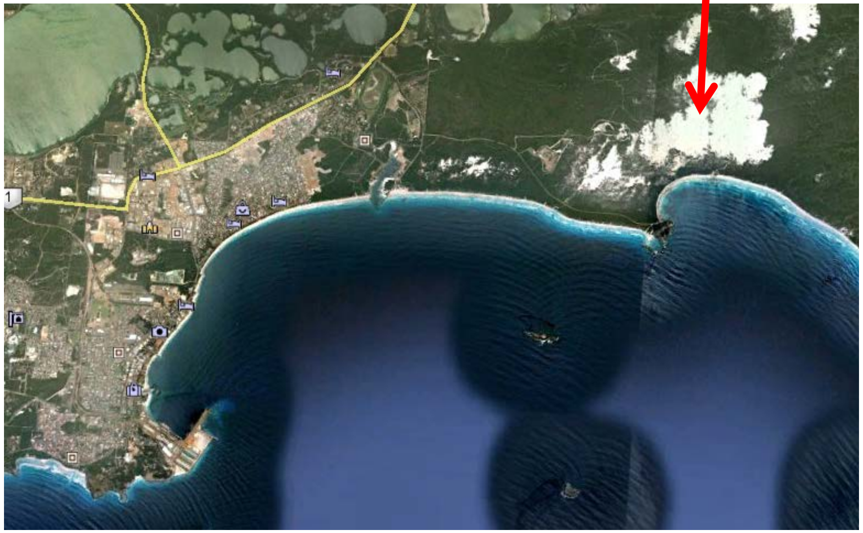
The sand sample is an ideal Internal Spectral Standard (ISS)

However

A common, an ideal homogenous and stable ISS sample in both time and (that can be shared with a large community) is not valid with the sand sample

Searching for an ideal standard took almost 4 years

Wiely Bay



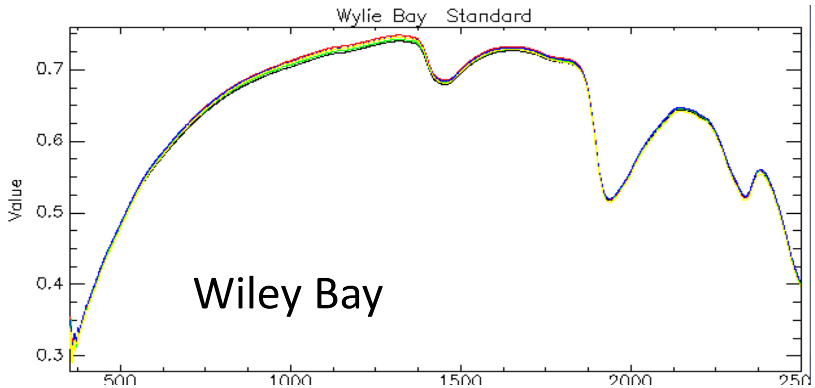
Lucky Bay

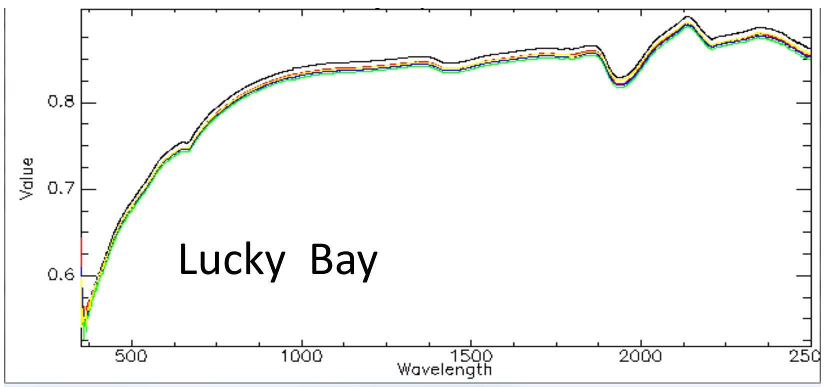
Lucky Bay

Wiely Bay

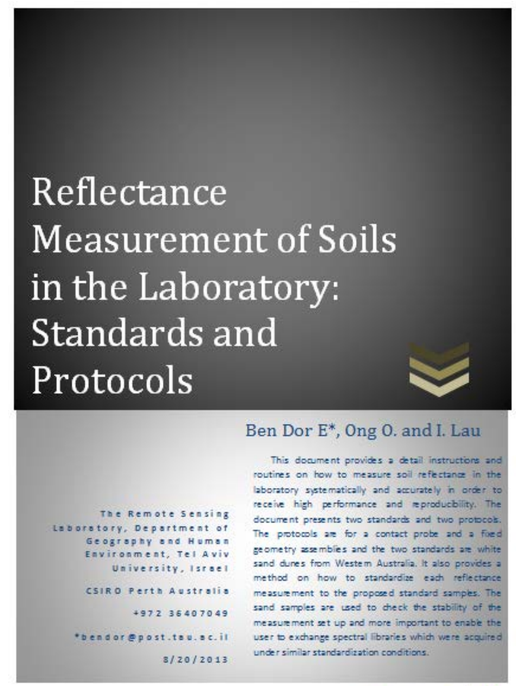
Lucky Bay **Wiely Bay**

50kg from each sample, washed and dried
More than 1000 samples available from each batch





XRD	Hig Moisture (several measurements over 6 weeks)
Quartz (90%), Aragonite (10%)	<0.1%
Quartz (100%)	<0.1%



Reflectance Measurement of Soils in the Laboratory: Standards and Protocols

Ben Dor E*, Ong O. and I. Lau

This document provides a detail instructions and routines on how to measure soil reflectance in the laboratory systematically and accurately in order to receive high performance and reproducibility. The document presents two standards and two protocols. The protocols are for a contact probe and a Fixed geometry assembles and the two standards are white sand dunes from Western Australia. It also provides a method on how to standardize each reflectance measurement to the proposed standard samples. The sand samples are used to check the stability of the measurement set up and more important to enable the user to exchange spectral libraries which were acquired under similar standardisation conditions.

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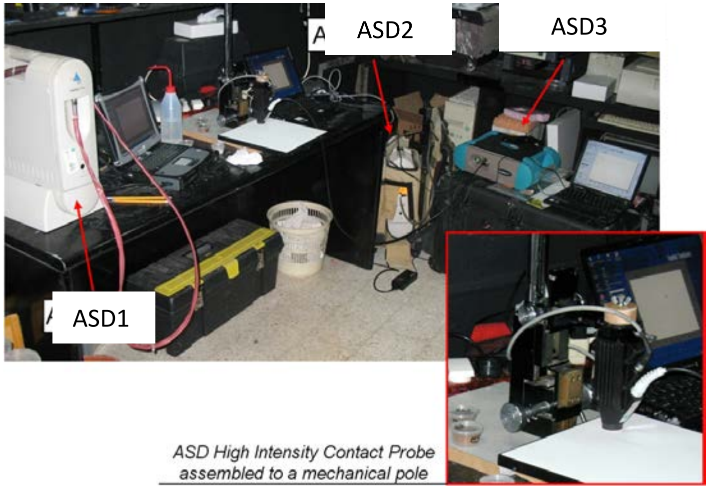
8/20/2013

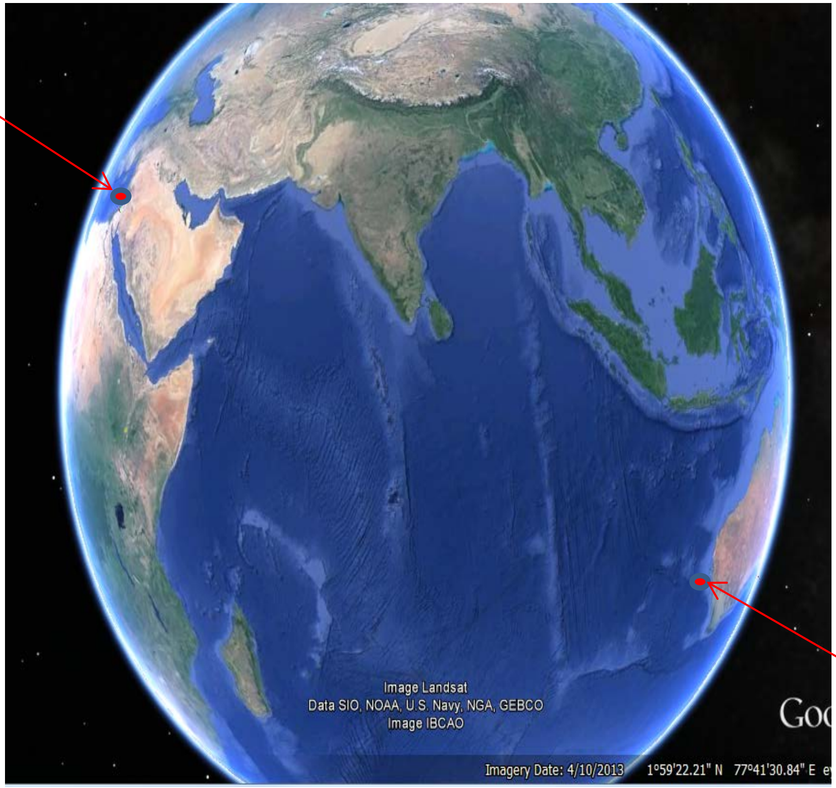
Five soils and different measurement conditions were used and corrected by the ISS approach using LB and WB samples

Sets Up



Tel Aviv

September



Perth

August

- 4 different protocols
- 5 different spectrometers
- 4 users
- 4 different White Reference
- 2 different geographical location

Same Soil Samples, Same ISS

CSIRO 0 - Brand New HALON Plate as a WR with, ASD-2, contact probe (CP), User-1, Perth, Protocol A(0) → **MASTER**

Results 1

Geoderma 245–246 (2015) 112–124

Contents lists available at ScienceDirect

Geoderma

journal homepage: www.elsevier.com/locate/geoderma

Reflectance measurements of soils in the laboratory: Standards and protocols

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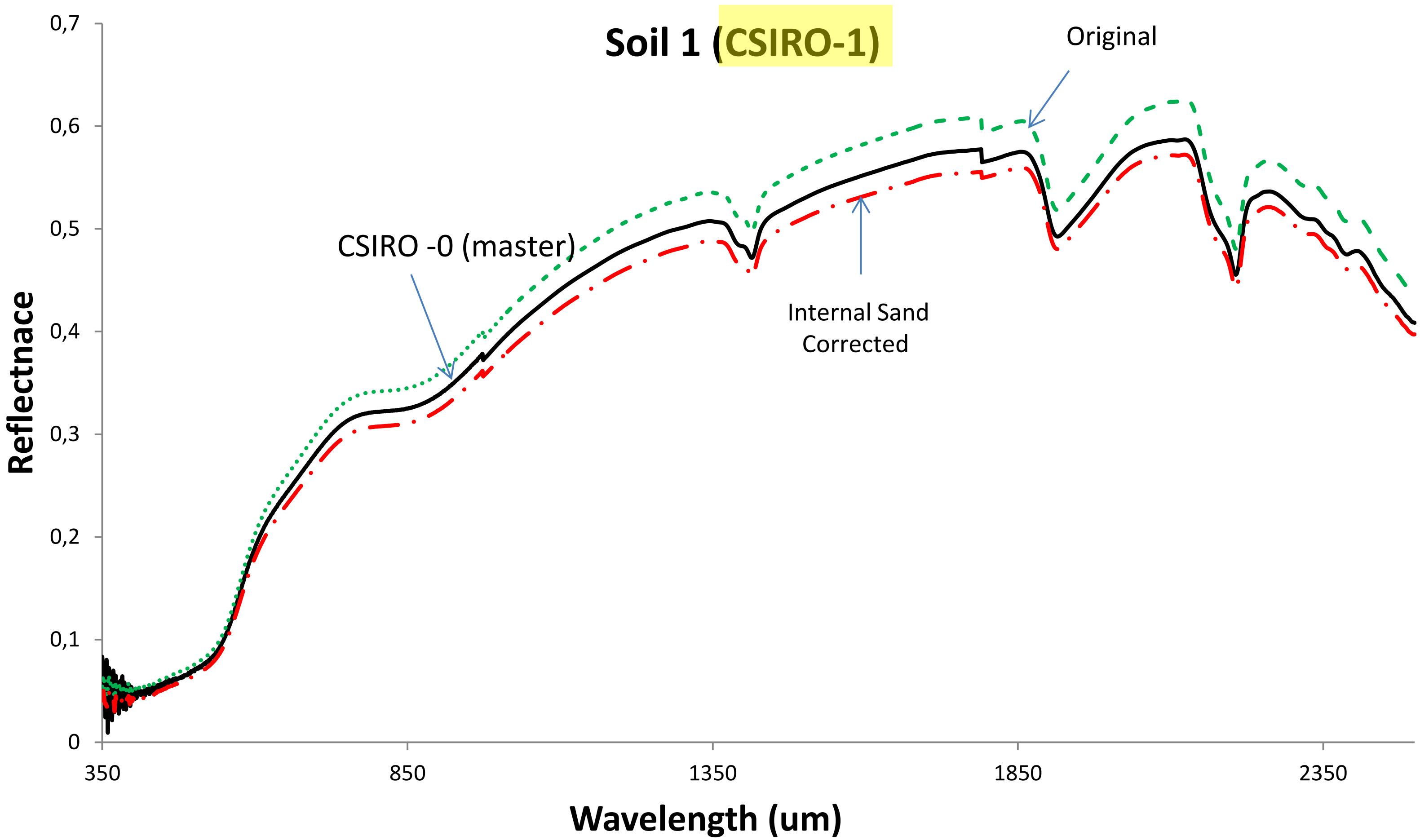
ARTICLE INFO

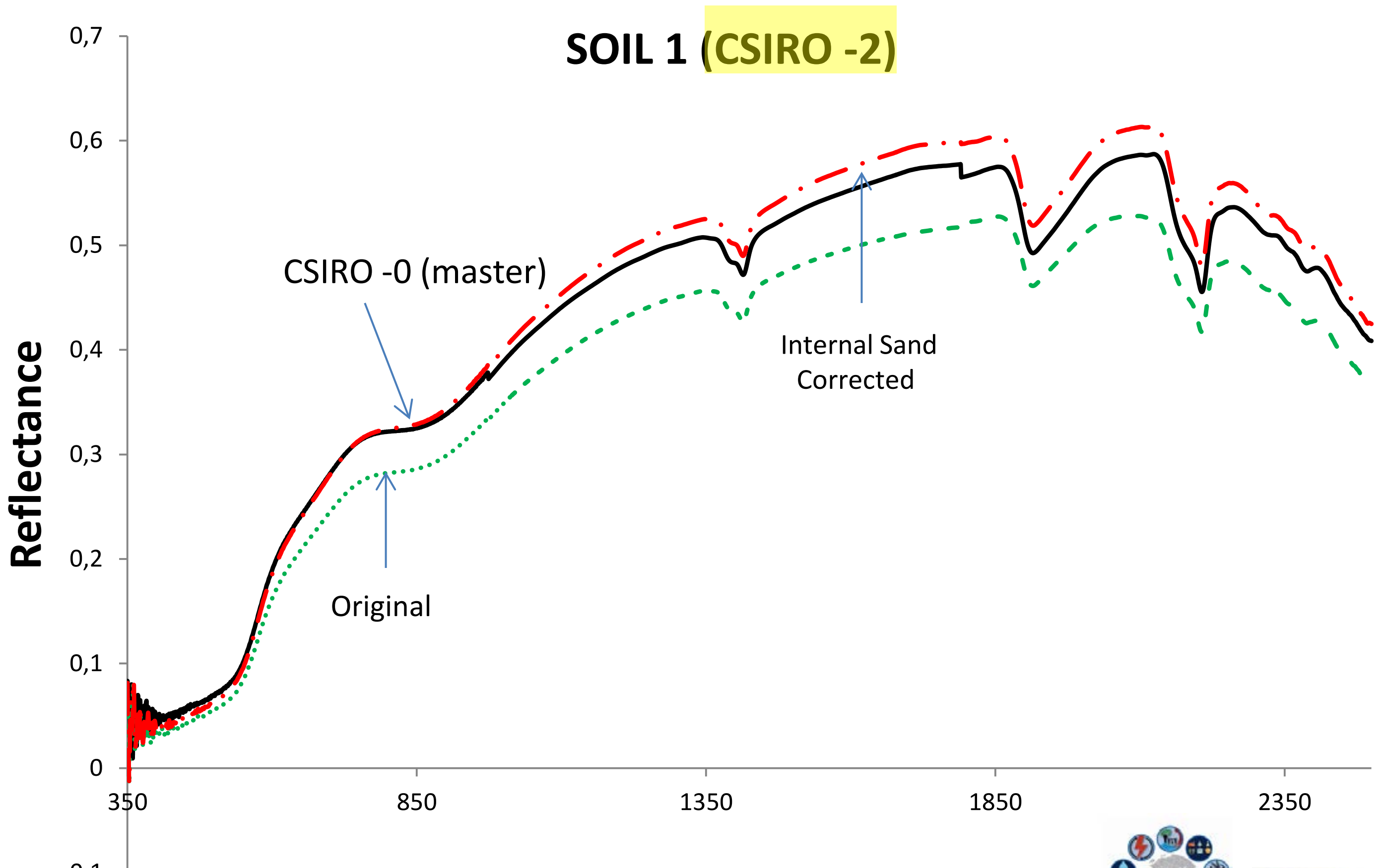
Article history:
Received 4 October 2014
Received in revised form 3 January 2015
Accepted 5 January 2015
Available online xxxx

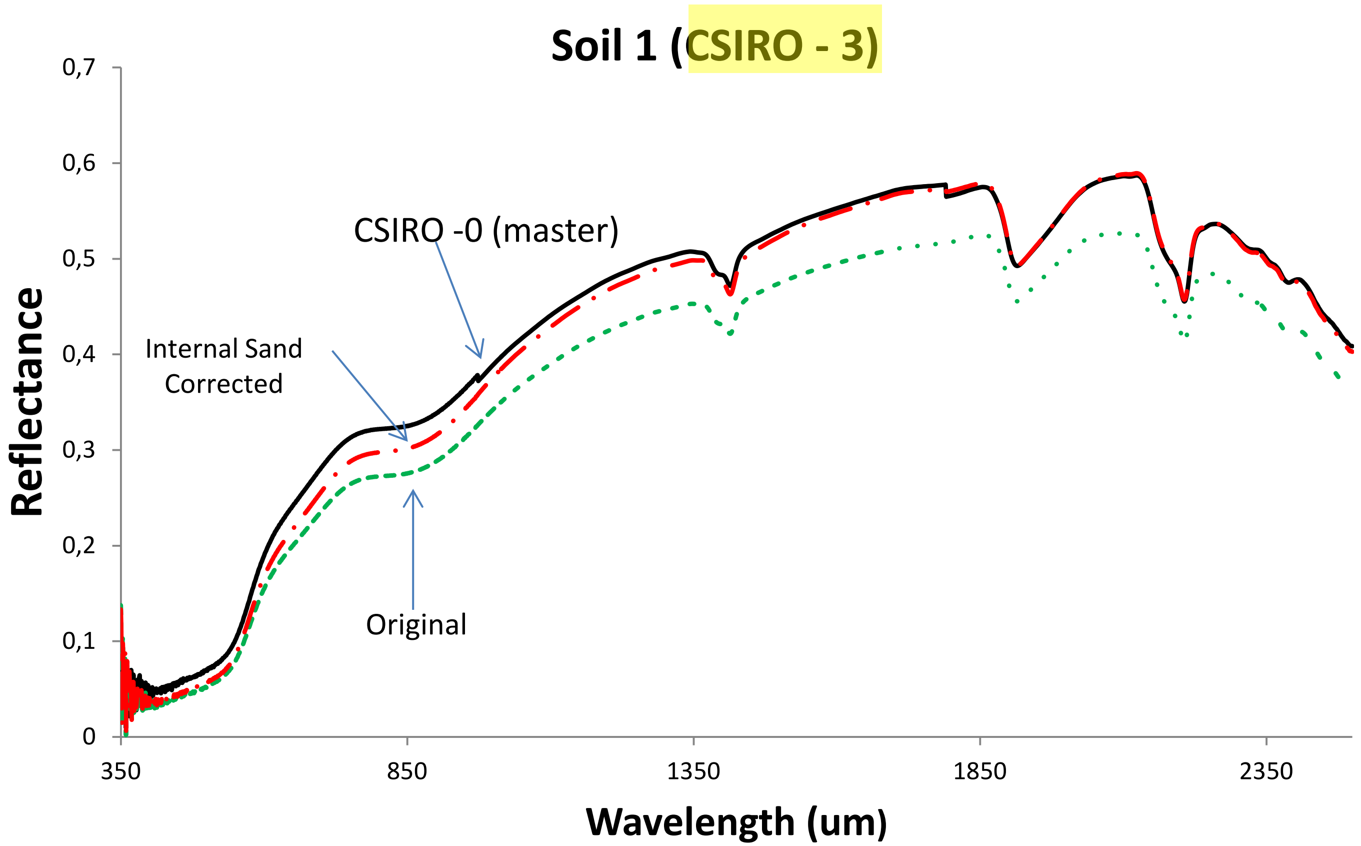
Keywords:
Soil spectroscopy

ABSTRACT

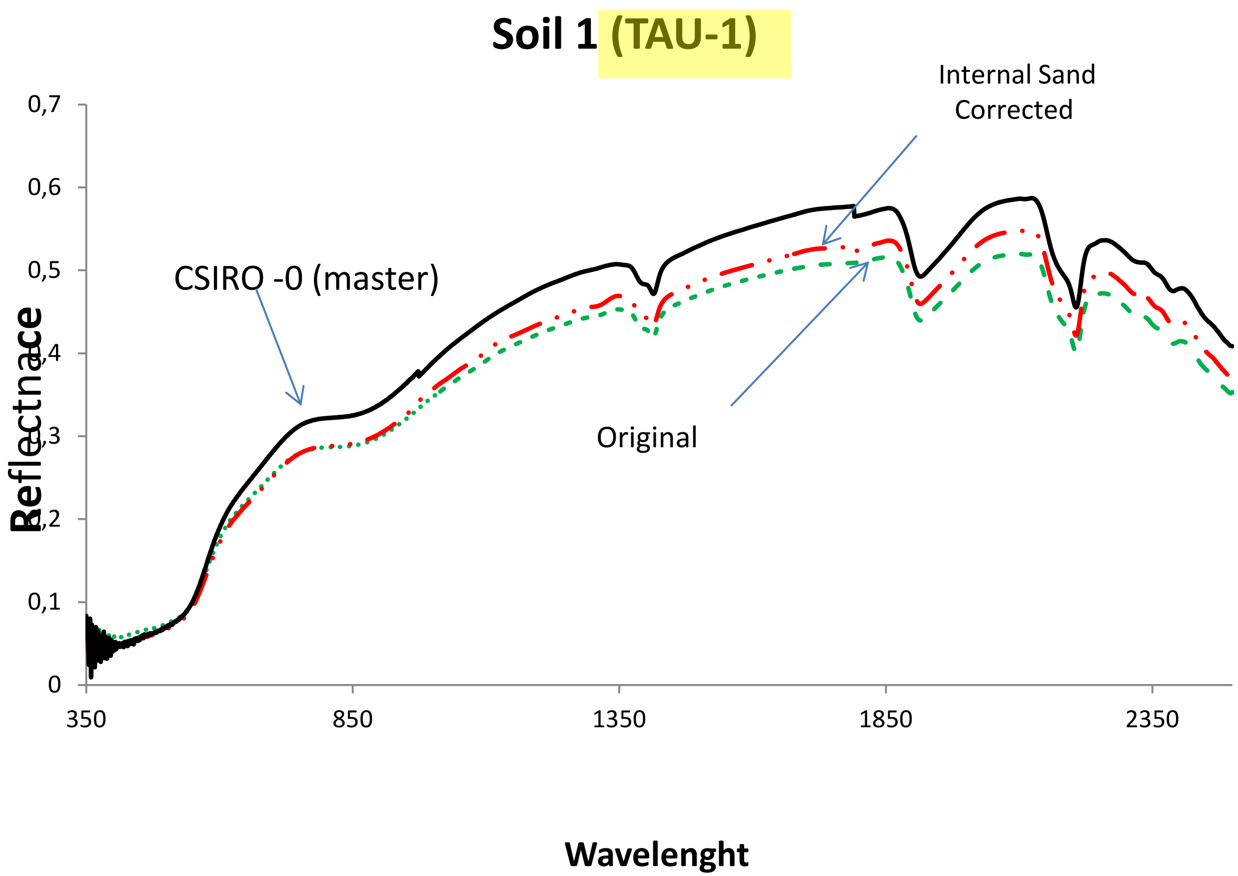
For the past 20 years, soil reflectance measurement in the laboratory has been a common and extensively used procedure. Based on soil spectroscopy, a proxy strategy using a chemometrics approach has been developed for soils, along with massive construction of soil spectral libraries worldwide. Surprisingly however, there are no agreed-upon standards or protocols for reliable reflectance measurements in the laboratory and field. Consequently, almost every user reconstructs his or her own protocol based on the literature, experience, convenience and infrastructure. This yields significant problems for comparing and sharing soil spectral data between users, as spectral variations can be encountered from one protocol to the next. This further prevents the generation of a robust model for a given soil property using the worldwide data archive. To solve this problem in the laboratory


Soil 1 (CSIRO-1)
Original
CSIRO -0 (master)
Internal Sand
Corrected
Reflectnace
0,7
0,6
0,5
0,4
0,3
0,2
0,1
0
350
850
1350
1850
2350
Wavelength (um)


SOIL 1 (CSIRO -2)
Reflectance
0,7
0,6
0,5
0,4
0,3
0,2
0,1
0
350
850
1350
1850
2350
CSIRO -0 (master)
Internal Sand
Corrected
Original



Soil 1 (CSIRO - 3)
0,7
0,6
0,5
0,4
0,3
0,2
0,1
0
Reflectance
350
850
1350
1850
2350
Wavelength (um)
CSIRO -0 (master)
Internal Sand
Corrected
Original


Soil 1 (TAU-1)
Internal Sand Corrected
CSIRO -0 (master)
Original
Reflectnace
Wavelenght
0,7
0,6
0,5
0,4
0,3
0,2
0,1
0
350
850
1350
1850
2350

ASDS = Average Sum of Deviation Square
(Ben-Dor et al., 2004)

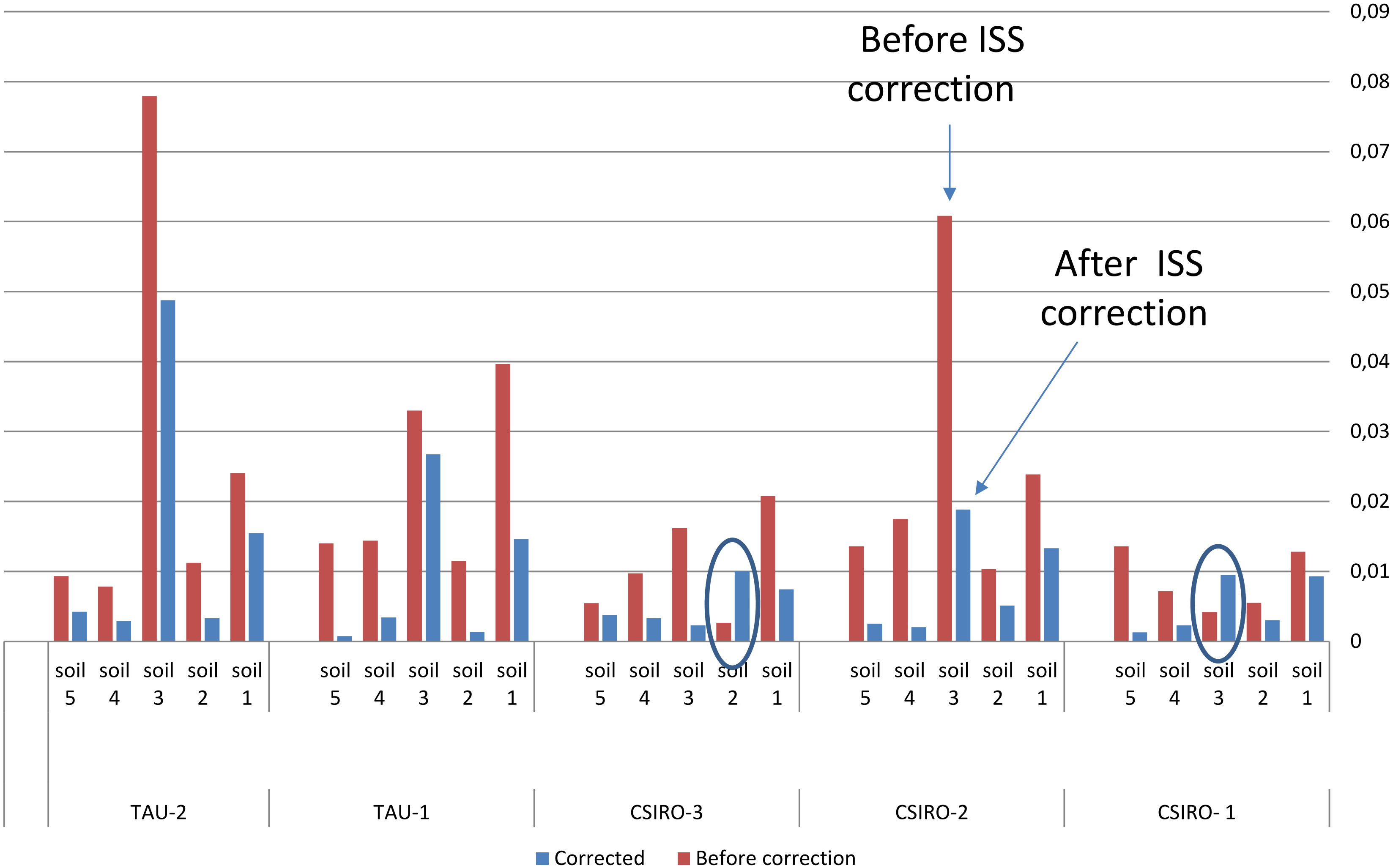
$$ASDS = \frac{\sum_{\lambda=350}^{2500} \sigma\left(1 - \rho_{\lambda} / \rho*_{\lambda}\right)^{2}}{2151}$$

ρ : sample reflectance
ρ * : reference reflectance

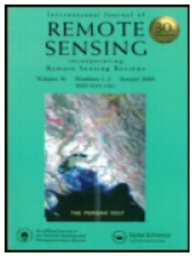
ASDS → 0 = good match

92% success

ASDS



Results 2



Taylor & Francis
Taylor & Francis Group

International Journal of Remote Sensing

ISSN: 0143-1161 (Print) 1366-5901 (Online) Journal homepage: http://www.tandfonline.com/loi/tres20

Normalizing reflectance from different spectrometers and protocols with an internal soil standard

Veronika Kopačková & Eyal Ben-Dor

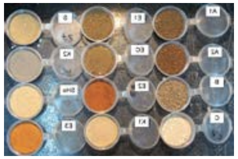
To cite this article: Veronika Kopačková & Eyal Ben-Dor (2016) Normalizing reflectance from different spectrometers and protocols with an internal soil standard, International Journal of Remote Sensing, 37:6, 1276-1290

To link to this article: http://dx.doi.org/10.1080/01431161.2016.1148291

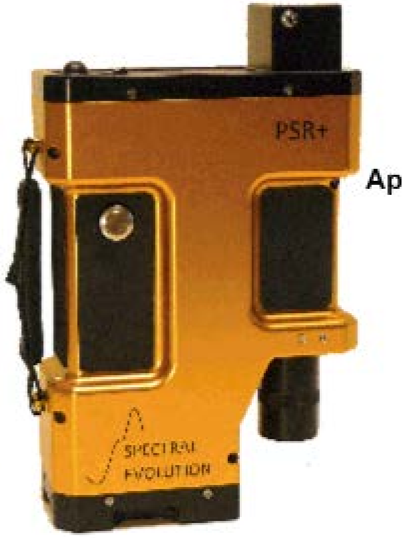
Validation Results (2015)

Czech Geology Society (CGS), Prague (SE) Tel Aviv University (TAU) Tel Aviv

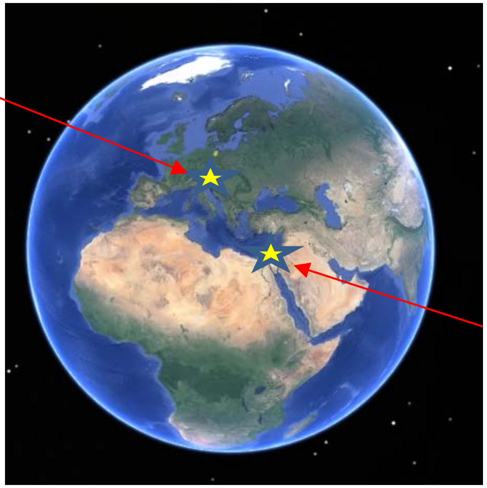
- Two different spectrometers make: ASD and Spectral Evolution
- 5 Australian soils + 10 Israeli soils



- Measured at TAU and CGS at different dates and different protocols
- The LB and WB were used as ISS samples at both locations



Spectral Evolution

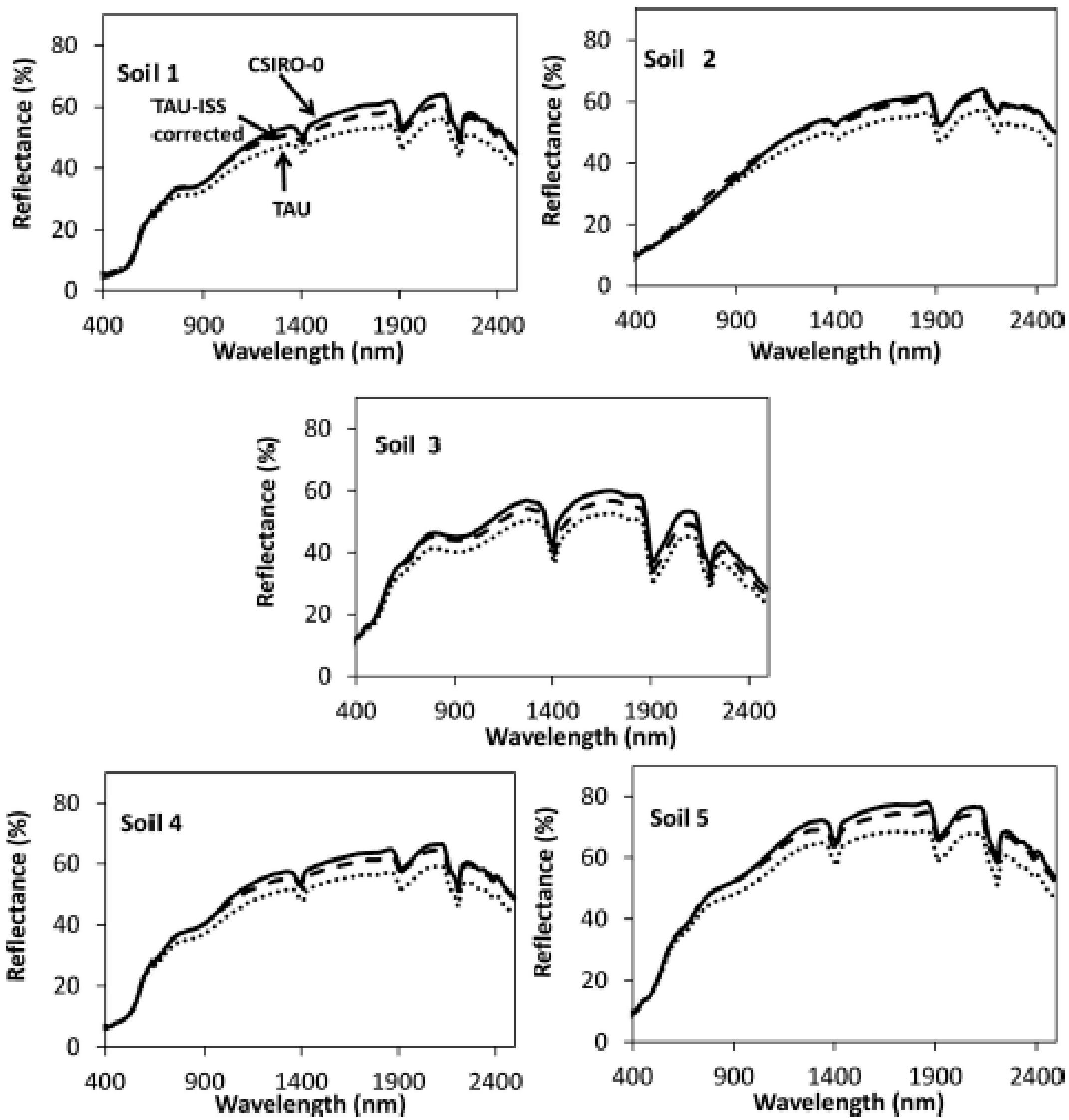


Prague

Tel Aviv

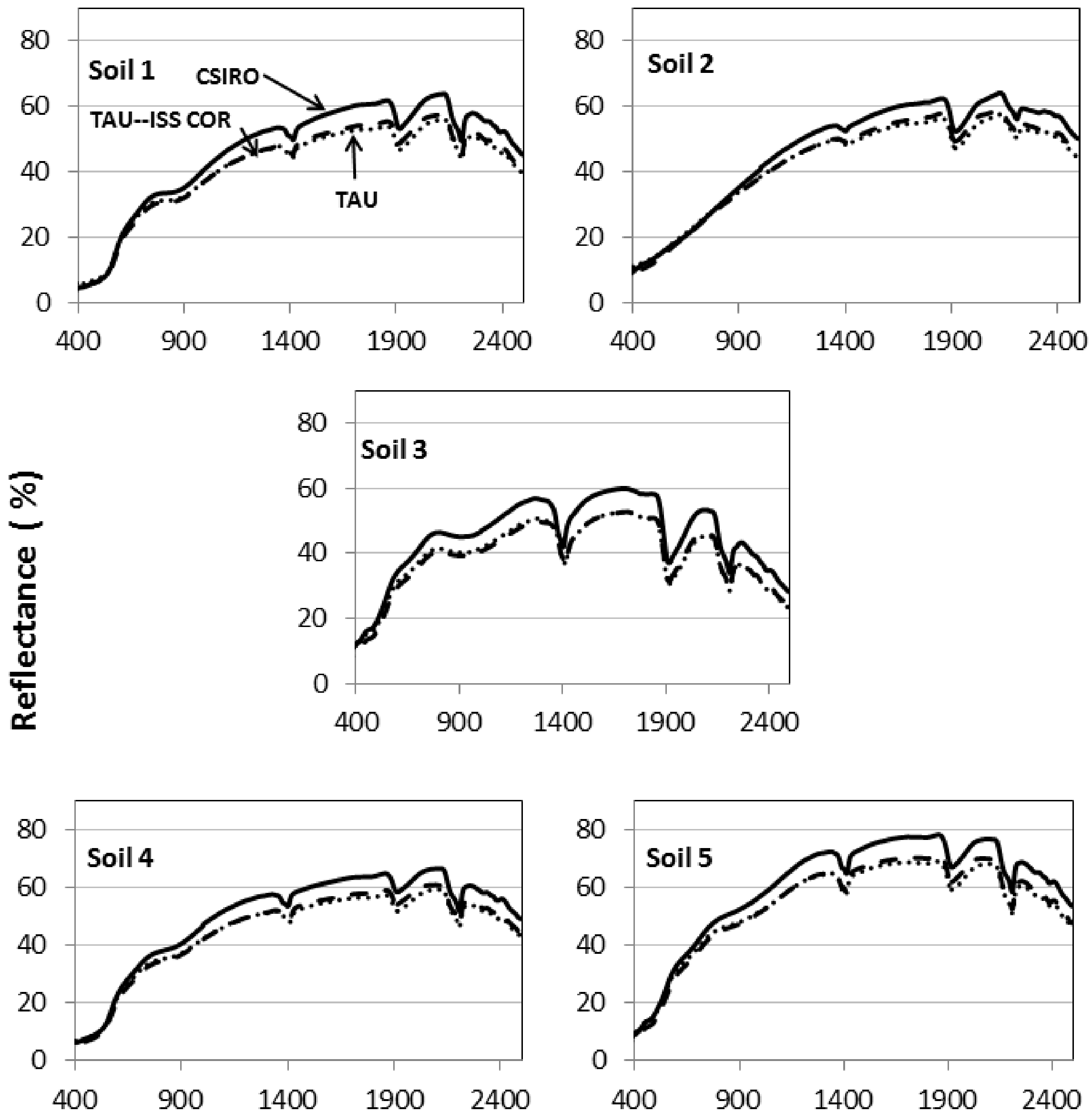
ASD

TAU **LB**



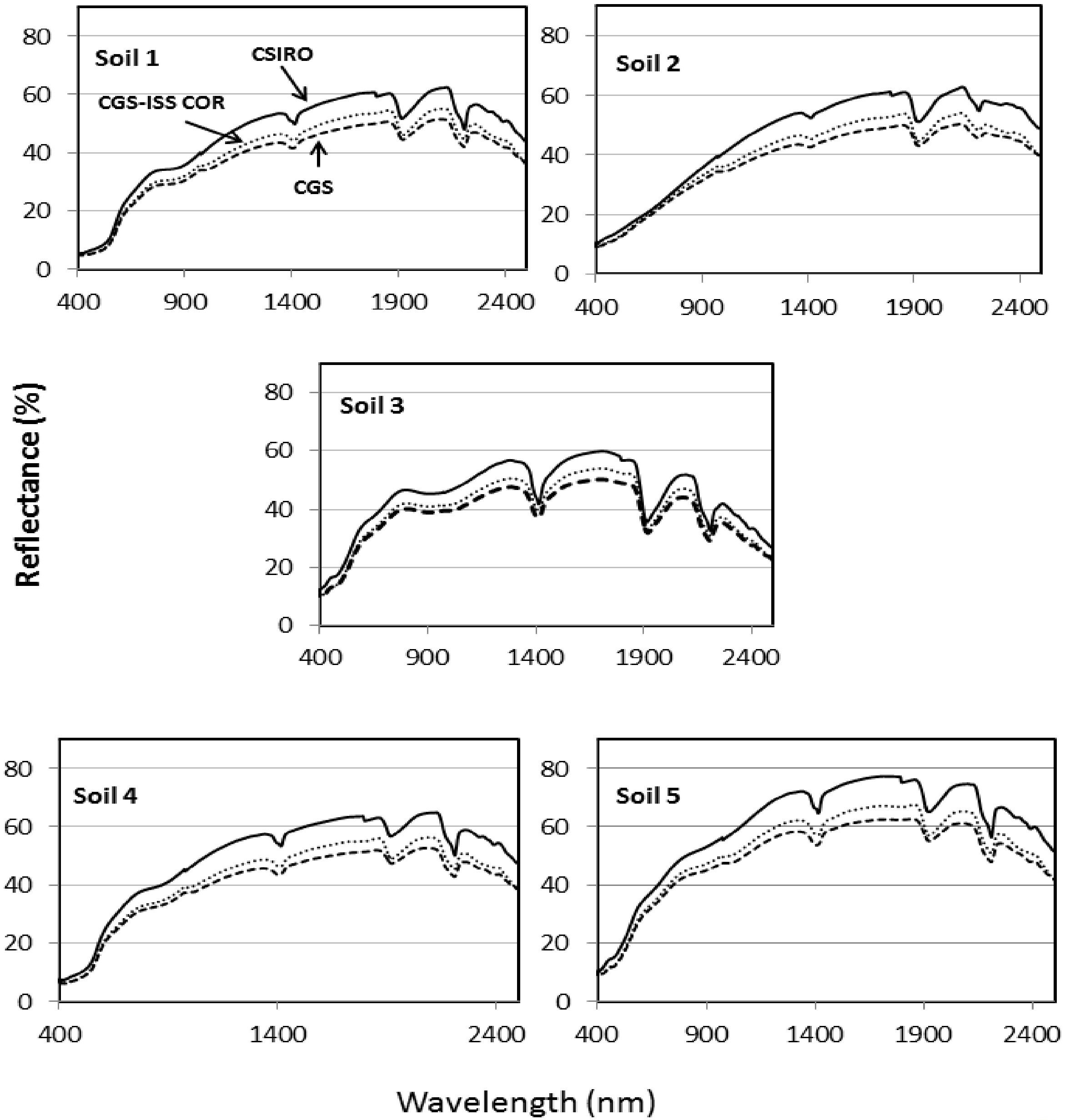
Soil 1
CSIRO-0
TAU-ISS corrected
TAU
Soil 2
Soil 3
Soil 4
Soil 5
Reflectance (%)
Wavelength (nm)
0
20
40
60
80
400
900
1400
1900
2400

TAU **WB**



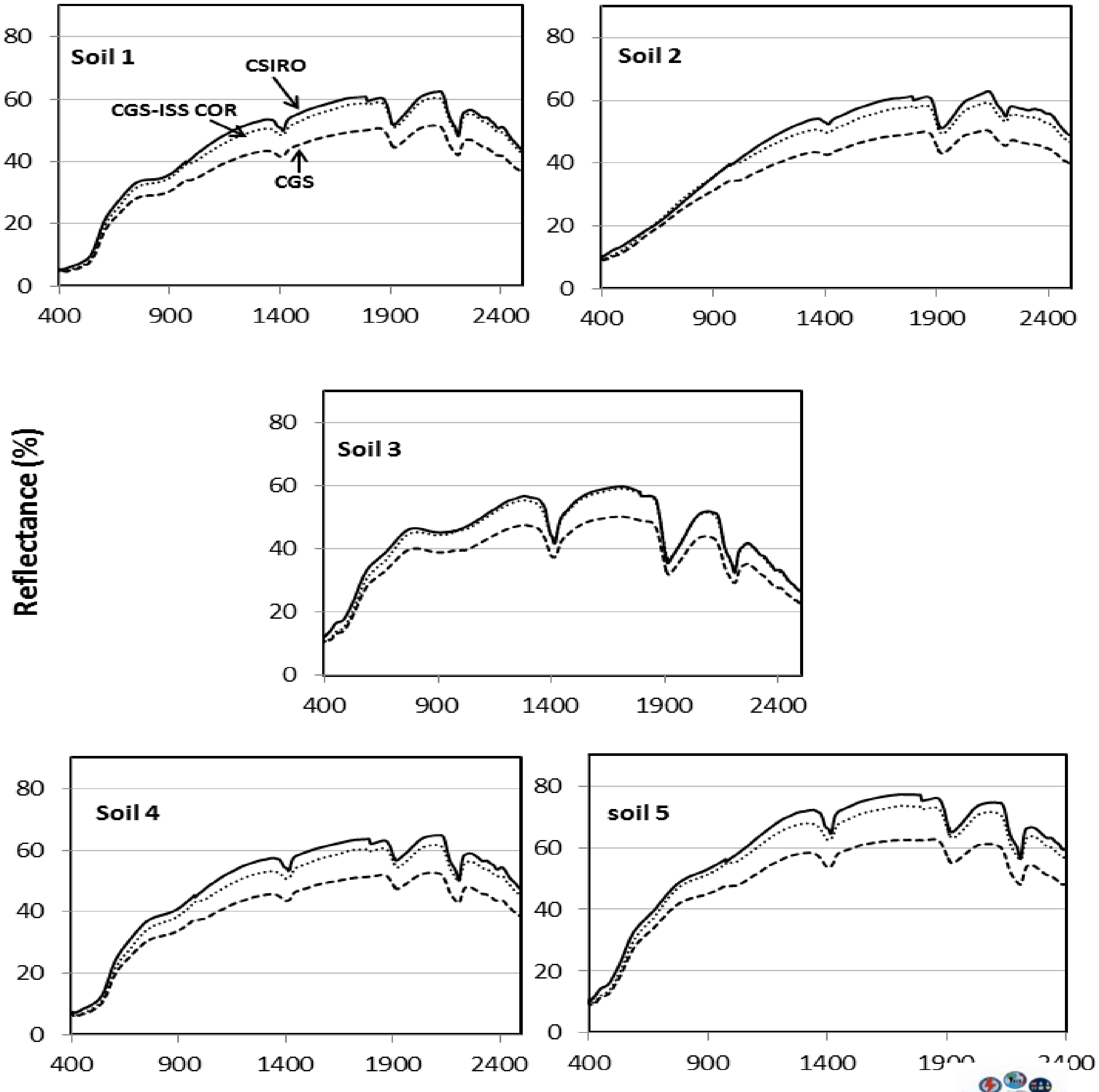
Reflectance (%)
Soil 1
CSIRO
TAU--ISS COR
TAU
Soil 2
Soil 3
Soil 4
Soil 5
80
60
40
20
0
400
900
1400
1900
2400

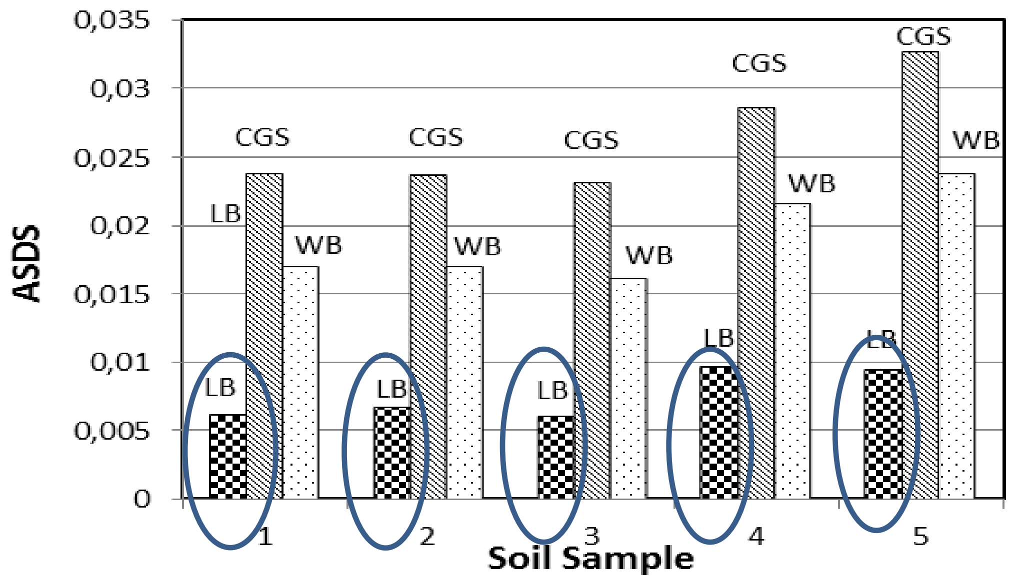
CGS **WB**

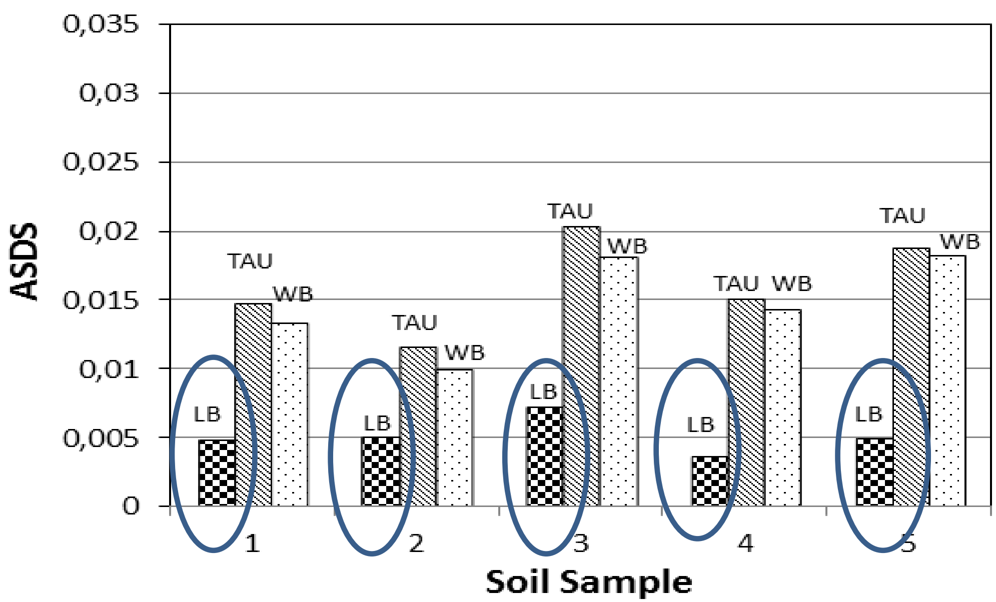


Soil 1
CSIRO
CGS-ISS COR
CGS
Soil 2
Soil 3
Soil 4
Soil 5
Reflectance (%)
Wavelength (nm)
80
60
40
20
0
400
900
1400
1900
2400

CGS **LB**


Soil 1
CSIRO
CGS-ISS COR
CGS
Soil 2
Soil 3
Soil 4
soil 5
Reflectance (%)
0
20
40
60
80
400
900
1400
1900
2400





LB is a best performing sample

Recent Results

The Analytic Aspect

Česká zemědělská univerzita v Praze

- 72 Soil samples were measured at Czech University of Life Science (CULS), Prof Luboš Borůvka using the CUL protocol
- The same soil samples were measured at TAU using CSIRO protocol with **LB** ISS

Marked are the highest values of statistical parameters

The two data sets were identical analyzed by PARACUDA II

max	CalR2	TestR2	RPD	SEP		CalR2	TestR2	RPD	SEP
Cox	0.971107	0.947636	4.341924	0.093856		0.965478	0.954473	4.560105	0.084314
pH H20	0.89206	0.749738	2.199049	0.245551		0.872632	0.777645	2.289335	0.297937
pH KCl	0.977148	0.944391	4.588273	0.064873		0.971125	0.957072	5.452361	0.071309
Fed	0.858187	0.913769	3.334864	0.248033		0.916304	0.874774	3.172813	0.240496
Feox	0.986081	0.911705	3.182581	5.847144		0.975933	0.959098	4.846087	3.654969
Mnd	0.977608	0.887721	3.202772	324.9865		0.953391	0.832919	2.760402	313.978
Mnox	0.945616	0.951499	4.155613	0.243106		0.949423	0.90411	2.97882	0.364531

CULS TAU

Accuracy: no significant difference between CUL and TAU protocol

As long as any protocol is kept – accuracy is preserved

ISS is more for SSL exchange and for sensor stability and cross calibration aspects

Groups who are using the ISS so far:

1) Czech Geology Survey, Czech Republic
2) i-BEC Greek
3) TAU Israel
4) University of Sao Paulo Brazil
5) GFZ -Potsdam
6) CSIRO Australia

Others are strongly encouraged

WP4 – Pilots towards Regional Challenges

Goal: Address the opportunities where *current* infrastructure (as identified in WP200) can be re-applied to address the gaps identified in WP3. Implementation of the action plan detailed in T3.3 Main pillars:

1. Climate Change
2. Food Security
3. Raw Materials
4. Energy

T4.2 – Soil Spectroscopy to improve Food Security

Our aim in GEO-CRDALE :

- To disseminate the SSL and ISS knowledge to North Africa, Middle Est and Balkan countries for establishing a regional SSL (workshop and summer school)

GROUP ON EARTH OBSERVATIONS

- To find users who are interested in EO for food security and share existing knowhow (survey and interview)

EUFAR GFZ Helmholtz-Zentrum Potsdam

Implementation of Soil Spectroscopy for digital mapping and monitoring of soils: Toward space applications and Transfer Technology Office (TTO) activities

EUFAR2 - EWG 4 "Hyperspectal Remote Sensing" and EWG-TTO

Workshop

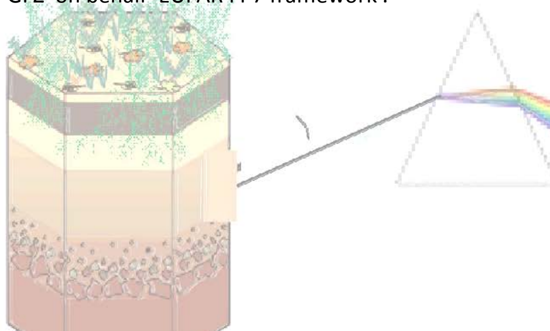
September 28-29, 2016

Potsdam, Germany

General:

An executive workshop on SOIL SPECTRAL LIBRARY (SSL) will be held on 28-29 Sep, 2016 in GFZ Potsdam Germany.

The Workshop is organized by the Remote sensing LAB at TAU and the Section 1.4 Remote Sensing at GFZ on behalf EUFAR FP7 framework .



The Motivation:

To gather expert and young scientists in hyperspectral remote sensing of soil in order to present, discuss and find the ways how to exploit the technology to support, in a credible manner, digital mapping and monitoring of soils. The emphasis will be placed on current hot topics related to 1) development of soil spectral libraries and standardization of protocols, 2) commercial applications, and 3) space applications and tools for prediction of soil properties

Registration :

Application with CV for the workshop must be email to the Workshop's chairs

The workshop is limited for 20 participants and not open for the public.

EUFAR will cover limited number of travel expenses and 2 nights

Acceptance policy

Young PhD and post-doc candidates who has a proven background in soil spectroscopy (preferable experience in SSL activity) and those who commit to initiate SSL activity at there home institute

Workshop guests :

Prof. Jose Dematte from University of Sao Paulo, Brazil , Dr. Raphael Viscarra Rossel from CSIRO Australia, Dr. Philip pe Lagacherie From INRA.

Special dates:

Pre-registration: July 30

Notification: August 30

Send CV to : bendor@post.tau.ac.il
chabri@gfz-potsdam.de

Workshop Chairs: Eyal Ben Dor (Tel Aviv University) and Sabine Chabrillat (GFZ)

A Workshop on behalf of EUFAR to the young soil spectral community for building SSL at their home institute according to the last standards and share information to enlarge the World SSL

September 28-29 GFZ Potsdam Germany

General Conclusion

- The Internal Sand Standard (ISS) is working and **correcting for both albedo and unrecognized spectral features** with out the need of using a (same) white reference. It also helps to **monitor the measurement's** stability and procedure.

- The Soil Spectral community is encouraged to adopt the ISS procedure (CSIRO protocol is recommended but not mandatory)

Recommendations and action items

- Send request (and get) LB sample + CSIRO-0 Spectra resampled to your spectrometer at: bendor@post.tau.ac.il.

- Fill in the GEO-CRADLE survey at: : http://geocradle.eu/index.php/inventories/capacities/gc-survey1

Thank to

The GEO-CRADLE project has received funding from the **European Union's Horizon 2020** research and innovation programme under grant agreement No 690133."

THE REMOTE SENSING LABORATORIES

Thank you for your Attentions

7TH GLOBAL DIGITAL SOIL MAPPING WORKSHOP 2016

GEO CRADLE

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