The acquisition and processing of voluminous spectral reflectance measurements of soils and powders for national datasets

IGARSS 2017 - Fort Worth, Texas, USA

Ian C Lau, Cindy C H Ong, Carsten Laukamp, Patrice de Caritat, Matilda Thomas

27th of July 2017

2 Geoscience Australia
Introduction: Collection of large spectral datasets

- National database of >1300 soil samples from across Australia, which had been chemistry analysed.
- Publicly available spectral data to compliment the geochemistry and soil properties.
- Develop a method to collect, capture and deliver a large spectral dataset with the associated data.
- Standardized method of collection for other projects.
Patrice de Caritat, Geoscience Australia

Sampling conducted in collaboration with the State and Territory Geological Surveys.

Initiated due to lack of geochemical coverage available for Australia and because such a data layer is fundamental to successful mineral exploration.

Transported regolith samples at the outlet of large catchments.

Sampled at two depths:
- 0-10 cm below the surface;
- 60 and 80 cm depth.

1390 catchments covering 91% of Australia.

Samples were dried, riffle split and sieved >2000 µm.

60 elements using mainly XRF and collision cell ICP-MS.

Archival of split of each bulk sample.
Instrumentation

- **Visible-near-shortwave infrared**
  - Panalytical ASD FieldSpec4 with high intensity contact probe.
  - Labsphere 99% Spectralon (PTFE) reflectance standard (2 inch round).
  - Lab jack and retort stand.

- **Mid-longwave infrared**
  - Bruker Vertex 70 and 80v FTIR spectrometer.
    - KBr beam splitter
  - Bruker A562 gold coated integrating sphere.
  - MCT detector with 2mm area.
  - Bruker integrating sphere sample cups (25 mm diameter, 3mm deep).

- **Software**
  - RS3, ViewSpec Pro, TSG
  - OPUS,
  - SPECCHIO.

Voluminous spectral reflectance measurements | Ian C Lau
Standards

- Lucky Bay (Western Australia) beach sand (quartz)
- Clay Mineral Society KGa-1b Washington County, Georgia, USA well crystalline Kaolinite
- Bruker diffuse gold coated reference

- Wavelength checking
  - REE doped Spectralon
  - HgAr lamp
  - Mylar
  - CO₂ and H₂O gases
Method

- Spectrometer preparation
- Sample preparation
- Measurement
- QA
- Processing
- Archiving
Voluminous spectral reflectance measurements | Ian C. Lau
Examples of NGSA soil spectra
Processing

- VNIR-SWIR
  - Step-correction
  - Relative to Absolute reflectance (using Spectralon calibration file)
- FTIR
  - Subsetting to remove long wavelength noisy data (>500 cm\(^{-1}\))
  - Export Bruker binary files as ASCII
  - Wavenumber to nanometre conversion
  - Resampling (if required)
- Import into The Spectral Geologist version 8.
- Mineral scalars processing
Quality control

- Visual
- SNR
- File naming (and time of acquisition)
- FTIR signal on the gold reference check
- Reference sample measurement – comparison with past measurements
- Gas absorptions in FTIR

KGa-1b Kaolinite

Lucky Bay quartz sand
QC Standards

- Checking of standards.
- Both instruments.
- Multiple measurement of standards each day.
Metadata

- Records for each set of measurements

This file lists all samples of the NGSA samples, measured by M. Thomas at the ARRC in Jan 2016

Supervision: Ian Lau

June 2013 and Jan 2014 samples were rescanned with Bruker 70 and ASD FieldSpec 4 due to time and wavelength differences. The remaining samples which had not been scanned previously were also started to be scanned, from 0000.

Location of raw data:
location of data acquired using Bruker Vertex 70 Integrating Hemisphere SWIR/MIR/TIR: \Swa1-perICEM-Share1C3DMMBRUKER FTIR data\NGSA\Australian_Soil_Project\NGSA_measurements_Jan2016\Bruker
location of ASD data corresponding to Bruker Vertex measurements: \Swa1-perICEM-Share1C3DMMBRUKER FTIR data\NGSA\Australian_Soil_Project\NGSA_measurements_Jan2016\ASD files

Total number of NGSA samples measured: 72.
Archiving of spectral data

- **Current:**
  - CSIRO Data Access Portal
    - [http://doi.org/10.4225/08/58af8e1c23237](http://doi.org/10.4225/08/58af8e1c23237)
    - ASCII (CSV) files for ASD and FTIR data
  - SPECCHIO Spectral Information System
    - Individual spectra with metadata and associated NGSA data

- **Future:**
  - Auscope Discovery Portal
  - Australian Geoscience Datacube
Problems encountered

- Use of different spectrometers (both VNIR-SWIR and FTIR) and detectors.
- Missed samples.
- Stray light in laboratory.
- Dirty Spectralon/poor panel placement.
- Non-vacuum sphere (atmospheric gas).
- Condensation on MCT detector after filling dewar.
- Consistency with packing samples in to sample holder.
- Grain size (sample texture) variations.
- A562 integrating sphere design characteristics.
Lessons learnt

◦ Dedicated spectrometers and accessories to a campaign.
◦ Consistent use of same white reference and maintaining it to a high standard.
◦ Record detailed metadata (white reference, instruments, operator, lab conditions).
◦ Regular QA of data (daily at a minimum)
◦ Regular reference sample measurement for QC (multiple daily).
◦ Archive spectra and meta data regularly.
Example

ASTER geoscience map validation using NGSA spectral data
NGSA $\text{Si}_{\text{XRF}}$ and ASTER Silica Index

Silica index
- Not quartz
- Quartz
- Sand

ASTER Silica Index (B13/B10)

$R^2 = 0.52$

Silica Index B13/B10

DHR convolved ASTER

NGSA geochem Si
- 0.000000 - 178160.226971
- 178374.000000 - 320890.718225
- 320907.000000 - 360018.832920
- 360295.000000 - 394552.958439
- 394607.000000 - 427819.776601
- 427951.000000 - 444453.185681
- 445091.000000 - 462661.000000