AfSIS Technical Specifications

Soil Health Surveillance



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Overview

The Africa Soil Information Service (AfSIS), a collaborative project led by the Tropical Soil Biology and Fertility Institute (TSBF) of the International Center for Tropical Agriculture (CIAT), based in Nairobi, will attempt to narrow sub-Saharan Africa's soil information gap and provide a consistent baseline for monitoring soil ecosystem services.

The AfSIS project area includes ~17.5 million km² of continental sub-Saharan Africa (SSA) and almost 0.6 million km² of Madagascar. This area that encompasses >90% of Africa's human population living in 42 countries. The project area excludes hot and cold desert regions based on the recently revised Köppen-Geiger climate classification, as well as the non-desert areas of Northern Africa, small island nations, protectorates and national territories.

The AfSIS ground survey teams are in the process of surveying and sampling this vast area using a spatially stratified, random sampling approach consisting of 60, 100 km² sentinel landscapes, which are statistically representative of the variability in climate, topography and vegetation of the project area.

Twenty-one of the 60 sentinel landscapes fall within biodiversity hotspots as designated by Conservation International. The main advantage of this new data collection effort lies in its hierarchical sampling approach that replicates soil and other biophysical (e.g., land cover) measurements at different spatial scales, linking consistent, georeferenced ground observations to laboratory measurements, agronomic field trials and remote sensing data.

Ground surveys of the AfSIS sentinel landscapes will provide ~9,600 new soil profile observations consisting of more than 38,000 individual soil samples. Georeferencing and sentinel landscape

documentation with digital photography will further ensure that sampling locations can be revisited at later points in time to quantify where specific changes occurred and which environmental and human-made factors caused these.

It would be cost and time prohibitive to analyze these new soil samples for e.g., carbon and nutrient content, texture, mineralogy, water holding capacity and an entire suite of other potentially important soil properties, using conventional laboratory techniques. Instead, a key innovation of AfSIS is to use both near and mid-infrared spectroscopy for soil analyses.

The new data collections will also be supported with data from what is currently the most comprehensive international soil profile database for Africa (see ISRIC WISE v. 3.1 at www.isric.org), which contains data on 4,173 African soil profiles. AfSIS will add to this resource by digitizing additional soil profile "legacy data" where these can be retrieved from African soil survey and research organizations, georeferenced and subjected to ISRIC's stringent data quality control criteria.

Substantial effort will be devoted to assembling and harmonizing satellite image time series and digital terrain models for SSA. These base maps will be used as spatial covariates for digital soil mapping, but can also be used for other mapping and modeling purposes. For example, AfSIS will use MODIS, Landsat, ASTER and Quickbird images and SRTM terrain models for soil mapping, land cover change detection and estimation of landscape carbon stocks. By linking legacy, field and laboratory data to remote sensing information, digital terrain models, and other existing environmental covariates, AfSIS will thus be able to provide a unique resource for producing a new generation of soil, vegetation and land-cover maps as well as wide range of statistical products for SSA.

Concepts of Soil Health Surveillance

Almost 70 years ago Hans Jenny outlined the dynamical systems framework of the state factors of soil formation for evaluating the condition of soils and in regulating the fluxes of energy, materials and organisms to and from them. The factors include climate, organisms, topography, parent material and time as well as more locally contingent variables such as fires, various forms of pollution, tillage, fertilizer applications, and livestock grazing, among others. As predicted by Jenny, human activities have dramatically altered the state of climate, organisms and the contingent factors on a global scale, and the rates of human-driven change processes are expected to accelerate over the next 100 years, particularly in Africa.

People depend on soils for a wide range of essential ecosystem services. For example, soils are a key resource in the production of food, forage, fuel and fiber. Soils store and cycle water from rainfall and irrigation and filter toxic substances through clay sorption and precipitation processes that determine surface and ground water quality. Soil organisms decompose organic materials, cycle nutrients and regulate gas fluxes to and from the atmosphere. As human populations have grown, there has been a strong tendency to trade off increases in the demand for provisioning services (e.g., for food and other commodities) for regulating (e.g., nutrient, greenhouse gas and hydrological cycling) and supporting services (e.g., biodiversity).

In many parts of sub-Saharan Africa (SSA), positive feedback dynamics between growing populations,

land cover and climate change have led to a rapid loss in the capacity of soils to deliver essential ecosystem services. In some instances this has initiated catastrophic ecological regime shifts, with prominent examples including the Lake Victoria Basin of East Africa, the Sahelian drylands and the humid forests of Madagascar.

These highly undesirable changes are not easily reversible and are major, though largely hidden, costs of development, which challenge the prospects of a better future for Africans, potentially leading to increased conflicts over land. Moreover, SSA's population is likely to double over the next 25-30 years, rising to an expected 1.75 billion people by 2050. This new population will not only demand more services from soils and ecosystems as a whole, but its per capita demand for such services must also increase if human development and poverty indices are to improve.

It is therefore striking that as humankind is successfully exploring, mapping, and monitoring other planets of our solar system, we know very little about the condition and trend of soils in Africa. In many African countries, soil data and maps have also vastly exceeded their expiration date, as state factors have changed dramatically since the 1960s and '70's, when many major soil surveys were conducted.

The state of the soil system is constantly changing, driven by small changes in individual soil properties. Important soil properties, often referred to as indicators, include soil organic carbon, nitrogen, acidity, color and so forth, while important drivers of these changes include soil climate, soil organisms and topography.

Soil health is often defined in the context of agricultural management or intervention. Kibblewhite et al. (2008), described soil health as an "integrative property that reflects the capacity of soil to respond to agricultural intervention, so that it continues to support both the agricultural production and the provision of other ecosystem services".

Fundamentally, soil health is often used to describe the general condition of the soil resource base. It integrates simultaneous function, is hence difficult to define precisely, and should not be confused with soil quality as used in the soil science community in recent decades. Quantifying soil health is not trivial given its integrative nature, and will not be possible using conventional indicators of soil fertility alone.

Some attempts have been made at developing indices for soil condition by using relatively novel approaches to the analysis of multivariate data and soil spectroscopic techniques (e.g. Vagen et al., 2006). In most situations establishing this relationship will require multivariate pattern recognition and calibration techniques.

Soil health surveillance in AfSIS is built around the use of new approaches to soil analysis which include soil infrared spectroscopic techniques, X-ray fluorescence, X-ray diffraction, and laser diffraction particle size analysis, as well as a range of statistical methods from multilevel modeling techniques to pattern recognition and machine learning.

Combing these analytical techniques allows for an integrative analysis of soil properties and the development of a holistic analysis of soil condition. For example, variables affecting soil nutrient capacity such as clay mineralogy, total elemental concentrations, absorbance spectra, texture and parent mate-

rial can be combined to provide a more accurate assessment of soils' nutrient capacity.

AfSIS employs this concept of soil health beyond agricultural landscapes and into semi-natural ecosystems, as native forests also require healthy soil for their productivity. This is also extremely important given current and historic land-change dynamics across the African continent. The idea is to provide an assessment of the soils' ability to provide essential ecosystem services, including, but not limited to agricultural productivity.

As mentioned above, there are many natural and human-induced drivers affecting soil condition. In order to understand the complex processes affecting soil productivity, soil degradation and overall soil condition, variables representing these drivers should also be monitored.

AfSIS employs a sampling methodology that attempts to understand and quantify factors affecting soil condition. This includes combining soil sample collection and analysis, with simultaneous measurements of vegetation type and structure, current and historic land use, visible erosion, and an analysis of satellite imagery, which allows for the incorporation of hydrologic patterns across the landscape, occurrence of fires and historic land-use change into the models. Combining these analyses allows for a more robust assessment of processes affecting soil condition, specifically identifying drivers of change and will ultimately aid in designing targeted restoration and preventive efforts.



2

Field Measurements

The field methods employed in the soil health component of the AfSIS project were developed at the World Agroforestry Centre, and are referred to as the Land Degradation Surveillance Framework (LDSF). The LDSF is designed to provide a biophysical baseline at landscape level, and a monitoring and evaluation framework for assessing processes of land degradation and the effectiveness of rehabilitation measures (recovery) over time.

The sampling framework is built around a hierarchical field survey and sampling protocol using sentinel sites that are 10×10 km in size (Figure 1). Each

sentinel site is stratified into 16 grid cells, and sampling cluster centroids are randomly located within the grid cells. Around each centroid, 10 sampling plots are randomly located covering an area of 1 km² (100 ha). Each sampling plot is 1000 m² (0.1 ha). Each sampling plot has 4 subplots (Figure 3), each of 100m². Observations and measurements are made either at the plot or subplot level.

The framework provides field protocols for measuring indicators of the "health" of an ecosystem, including vegetation cover, structure and floristic composition, historic land use, visible signs of soil



Figure 1. AfSIS sentinel site (blue dots are sampling plots) near Megwin, Ethiopia. The site is 10x10 km in size.

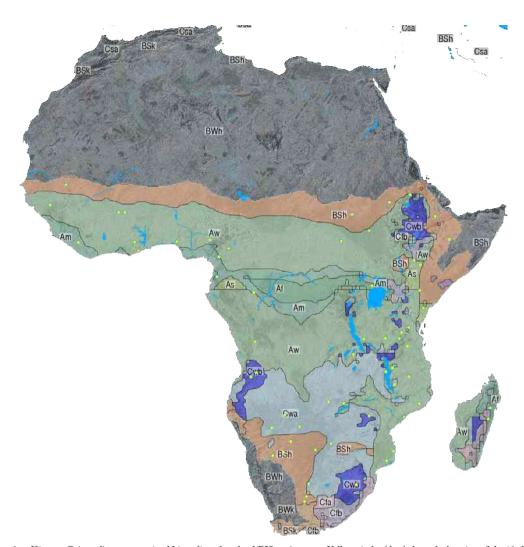


Figure 2. Köppen-Geiger climate zones in Africa, clipped to the AfSIS project area. Yellow circles (dots) show the location of the 60 AfSIS sentinel sites. Background is a topographical shading image based on the SRTM DEM.

degradation, and soil physical characteristics. A sampling framework for collection of soil samples is also provided, as described in more detail later. In AfSIS, sentinel sites represent a stratified random sample of landscapes in Africa south of the Sahara. The stratification is based on Koeppen-Geiger

climate zones (Figure 2 - http://koeppen-geiger. vu-wien.ac.at).

Sentinel sites may also be selected at random across a region or watershed, or they may represent areas of planned activities (interventions) or special interest.

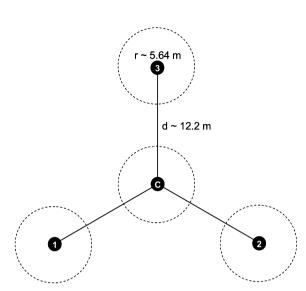
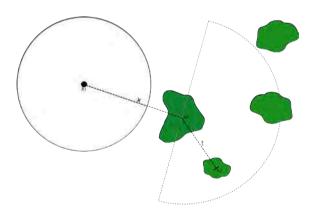


Figure 3. AfSIS plot $(1000 \, m^2)$ layout (radial arm), showing the four sub-plots (C,1,2,3 – each $100 \, m^2)$.



 $\label{thm:conditional} Figure~4.~~Sketch~illustrating~the~T\mbox{-}square~method~for~measurement} of~woody~cover~in~AfSIS~plots.$

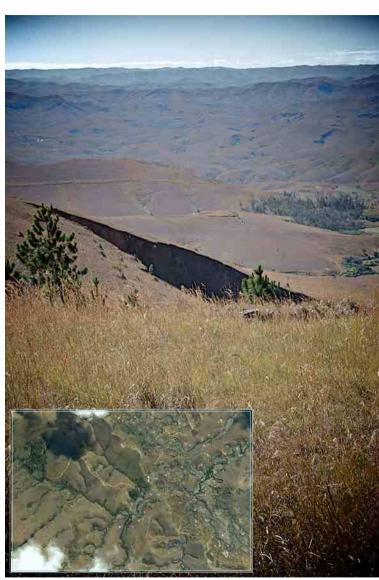


Figure 5. Lavaka erosion in the highlands of Madagascar. Photo was taken from the SW corner of the inset satellite image, looking NE.

2.1 Vegetation measurements

Woody- and herbaceous cover ratings are made using a Braun-Blanquet (Braun-Blanquet, 1928) vegetation rating scale from 0 (bare) to 5 (>65% cover). Woody plants (shrubs (<3 m height) and trees (>3 m height)) are counted at each subplot to obtain density estimates for trees and shrubs. Distance-based measurements are also carried out at each subplot using the T-square method (Krebs, 1989) (Figure 4) to determine vegetation distribution.

The "T-square" method is one of the most robust distance methods for sampling woody plant communities, particularly in forests, but also in rangelands. It can be used to estimate stand parameters such as distribution (random, non-random, clumped, non-clumped), density, basal area, biovolume, and depending on the availability of suitable allometric equations, also biomass. The LDSF field protocols have also been supplemented with destructive harvesting of trees.

The advantage of this method, over other commonly used distance methods such as the point-centered quarter (PCQ) method, is that it is less prone to bias where plants are not randomly distributed.

2.2 Soil field characterisation

Soil sampling

Top- and subsoil samples are collected from each subplot at 0-20 cm and 20-50 cm depth increments, respectively, and pooled (composited) into one sample for each plot and depth, resulting in a total of 320 standard soil samples per sentinel site. These samples are analyzed using NIR and MIR spectroscopy and a subset is subjected to reference analysis. (see page 20).



Figure 6. Measurement of soil infiltration capacity

Field texture

Top- and subsoil field texture is determined by hand using a ribbon test (Figure 7), and the ribbon length and feel are recorded in the field data entry form. Field texture is determined automatically in the database. Auger depth (root depth) restrictions are noted (in cm) if present during soil sampling.

Root Depth Restrictions

Auger depth (root depth) restrictions are recorded (in cm) if present during soil sampling.

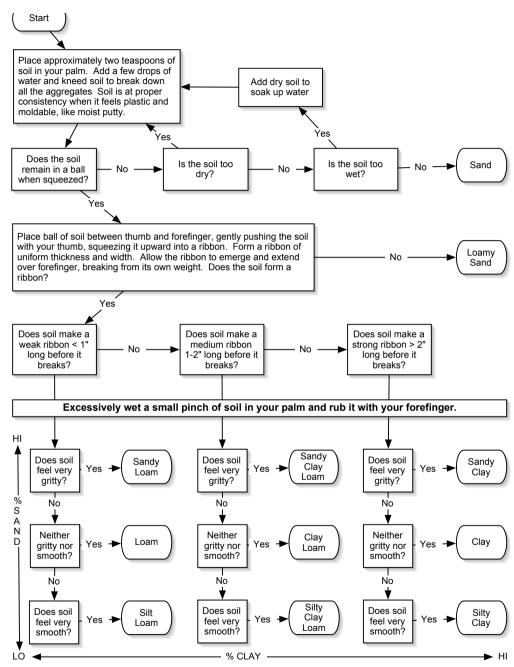


Figure 7. Soil texture by feel flow-chart.

Cumulative soil mass

Cumulative mass soil samples are collected to 100 cm (0-20, 20-50, 50-80, 80-100 cm) at all infiltration plots and plot one (1) of each cluster. Plot one is included because it is the reference plot and all soil samples from this plot are subjected to standard chemical and physical reference analyses to calibrate prediction models from IR spectra. No additional cumulative mass samples are taken.

Soil erosion by water

Water erosion results from the removal of soil material by flowing water. A part of the process is the detachment of soil material by the impact of raindrops. The soil material is suspended in runoff water and carried away. Four kinds of accelerated water erosion are commonly recognized: sheet, rill, gully, and tunnel (piping).

In each sub-plot (C, 1, 2, 3 - Figure 3), signs of visible erosion are recorded, including the dominant type of erosion, together with rock/stone/gravel cover on the soil surface.

Soil infiltration capacity

This is the most time-consuming aspect of the field methodology. It is generally desirable to obtain a minimum of 3 infiltration tests in each cluster, allocated randomly to the different plots in the cluster.

In AfSIS we use a single ring infiltration ring. The ring is placed at the center of the plot. The soil is pre-wet the soil with 2-3 liters of water, which left to soak in for at least 15-20 minutes.

The test is conducted by maintaining a constant head, and reading the level every 5 minutes for the first half hour of the test. After 30 minutes, readings are made every 10 or 15 minutes, for up to 2 hours.

2.3 Land cover classification

Land cover of all plots is recorded using a simplified version of the FAO Land Cover Classification System (LCCS), which has been developed in the context of the FAO-AFRICOVER project (http://www.africover.org).

The "binary phase" of LCCS recognizes 8 primary land cover types, only 5 of which are sampled, including:

- 1. cultivated and managed terrestrial areas,
- natural and semi-natural vegetation,
- 3. cultivated aquatic or regularly flooded areas,
- 4. natural or semi-natural aquatic or regularly flooded vegetation, and
- 5. bare areas.

Artificial surfaces and associated areas, natural and artificial water bodies, and surfaces covered by snow or ice are not formally surveyed in AfSIS, but their presence within a cluster should be noted and georeferenced.

The "modular-hierarchical phase" of LCCS further differentiates primary land cover systems on the basis of dominant vegetation life form (tree, shrub, herbaceous), cover, leaf phenology and morphology, and spatial and floristic aspect. All the associated features are assessed visually and are generally coded on either categorical or ordinal rating scales. The ratings can subsequently be converted to unique hierarchical identifiers representing different land cover types.

2.4 Soil biodiversity sampling

In a selection of AfSIS sentinel sites, soil biodiversity sampling is being conducted, focusing on soil macrofauna, which is the visible part of the belowground biodiversity among which termites, ants, and earthworms are referred to as ecosystem engineers due to their marked impact on soil function.

The soil system hosts a diverse community of soil organisms involved in several ecological functions and ecosystem services such as nutrient cycling, control of pest and diseases, organic matter decomposition and carbon sequestration, and maintenance of a soil structure (Lavelle et al., 2006).

Earthworms comprise 40-90% of the soil macrofaunal biomass in most ecosystems (Fragoso et al., 1999) and are sensitive to ecosystem disturbance (Fragoso et al., 1999; Decaens et al., 2002, Tondoh et al., 2007) and rehabilitation (Hole et al., 2005, Ortiz-Ceballos and Fragoso, 2004; Schmidt et al., 2003; Sepp et al., 2005). Consequently, they can be used as a potential indicator of changes in terrestrial ecosystems in the context of land degradation assessment. Earthworms have been selected as they are (i) responsive to a range of environmental stresses, and (ii) easily measured and quantified.

Earthworm sampling

Sampling should occur during the short or long rains, when individuals are most active and can be easily sampled (Tondoh and Lavelle, 2005).

In AfSIS sites where soil macrofauna is sampled, this is conducted in the plots where infiltration measurements are undertaken, as well as in two additional plots per cluster (5 plots per cluster). In total 80 sampling points are sampled per site.

Earthworms are collected using a 25 x 25 x 10 cm iron frame (Figure 8). A soil monolith is then delin-



Figure 8. Iron frame (right) and sampling jars for collecting earthworms (Kubease Sentinel Site, Ghana)

eated, excavated using a spade and kept in a tray in order to hand-sort earthworms. Specimens collected are preserved in 70% alcohol.

Earthworm identification

Earthworm samples taken to the laboratory are separated into morphotypes, genera or species using a binocular microscope whenever possible before being sent to the Hungarian Natural History Museum for confirmation or identification. Samples are kept in 4% formaldehyde after counting and weighing.

Data processing and analysis

Data collected is (i) converted to density (individuals m⁻²) and biomass (g m⁻²) to assess the variation of earthworm populations across land-use types, and (ii) species richness is estimated per site by extrapolation methods such as first-order Jacknife, second-order Jacknife, Chao, and ACE which are implemented in the free software EstimateS (Colwell, 2005; Colwell and Coddington, 1994) and, (iii) assessment of indicator species or species assemblages characterizing groups of ecosystems using the IndVal program (Drufrene and Legendre, 1997).

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3

Laboratory Measurements

3.1 Approach to soil characterization

The AfSIS soil analytical procedures emphasize the measurement of soil functional properties that determine soil health – the capacity of soil the capacity of land to sustain delivery of essential functions or ecosystem services, such as hydrological regulation, nutrient supply to plants, and nutrient retention (Swift & Shepherd, 2007; Robinson et al., 2009). The outputs of AfSIS could contribute substantially to the new concepts of natural capital and ecosystem services. Three classes of properties can be defined according to the degree to which they show dynamic properties and to which they are influenced by management:

- Slow, management insensitive. Intrinsic properties of soils that change only slowly with time, primarily in relation to soil forming factors.
 They are key determinant of intrinsic soil functional properties and therefore important to measure to describe spatial variation in soil functional capacity. Examples are mineralogy and particle size distribution. Of course in extreme cases, all properties can be affected by management, e.g. severe human-induced soil erosion.
- Slow, management sensitive. Key indicators or determinants of soil functions that are responsive to management over periods of several years. Soil organic matter content is a good

- example. These are the most useful variables for long-term monitoring of soil functional capacity as a reliable estimate can be obtained from a single measurement point in time.
- 3. Fast, management sensitive. These properties may be important for some soil functions but fluctuate rapidly (e.g. within a year) in response to climatic, hydrological and management conditions. These variables require frequent monitoring to develop an understanding of their behaviour and to obtain reliable estimates of average values. It is generally difficult and expensive to conduct such measurements in large area surveys. Examples are mineral nitrogen, microbial activity, topsoil macro-aggregation. Few fast variables are management insensitive.

At AfSIS sentinel sites, priority is given to measurement Category 2 variables above, i.e. 'slow' variables that change only slowly with time in response to management and edaphic factors (e.g. soil organic matter levels).

Soil testing under AfSIS is designed to meet diverse needs of different users (e.g. McLaughlin et al., 1999): diagnosis of soil constraints for agriculture, monitoring of trends in soil health, land capability for agriculture, soil testing for engineering and stabilization purposes, ecological and human health risk assessment; and prognostic testing to inform investment decisions (e.g. fertilizer rates, soil conditioners, soil drainage, soil conservation).

In order to deal with the large number of soil

samples needed to adopt a soil health surveillance approach, soil infrared diffuse reflectance spectroscopy is used as the primary soil characterization tool (Shepherd and Walsh, 2007). A double (two-phase) sampling approach is used, whereby all samples are spectrally characterized, and random subsets are selected for reference measurements. Reference measurements are standard laboratory measurement methods used for soil characterization. These are usually too time consuming and expensive to perform on large numbers (thousands) of samples.

Near infrared (NIR) spectral measurements are conducted through regional laboratories in eastern, southern and West Africa (Figure 9). The NIR spectral laboratory network uses standard instrumentation and standard operating procedures to ensure reproducibility of results among laboratories and over time. More specialized infrared spectral measurements and reference analyses are all conducted through the World Agroforestry Centre (ICRAF) Soil-Plant Spectral Diagnostics Laboratory facility in Nairobi to ensure consistency of methods. The ICRAF laboratory provides technical backstopping and quality control for the network of near infrared spectral laboratories.

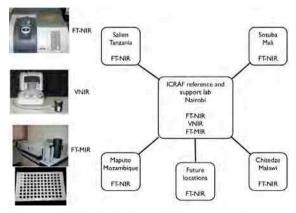


Figure 9. AfSIS soil infrared spectral laboratory network.



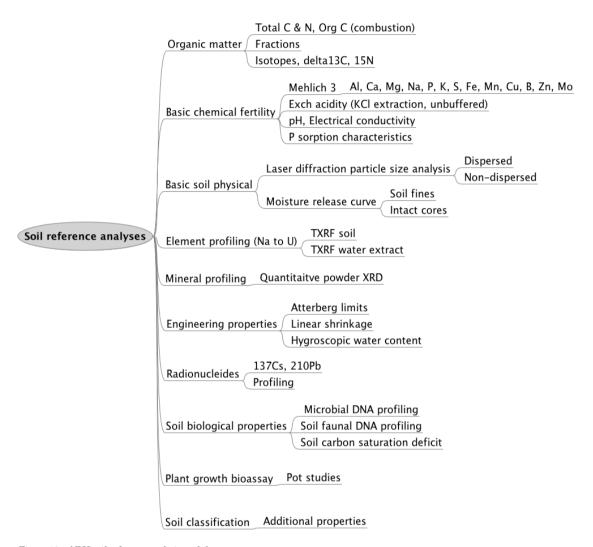


Figure 10. AfSIS soil reference analysis modules.

AfSIS uses a prioritized modular approach to soil reference measurements (Figure 10). The reference modules (e.g. standard soil fertility module) implemented and the size of subsample (i.e. number of samples) for reference measurements are constrained by available budget. At current funding levels, reference analysis modules are implemented

on a subsample of about 10% of all standard soil samples (32 samples per sentinel site).

Reference analyses that are more time consuming and expensive (e.g. stable isotope analysis) are conducted on smaller subsets of samples than cheaper faster reference measurements. Currently proposed modules are described below, but additional modules may be added according to special interests of other projects.

Legacy soil samples are also included where these can be obtained. These are restricted to samples that are georeferenced, have soil profile descriptions, and have been stored in good condition (e.g. Sheppard and Addison, 2008) with clear labeling.

Standard operating procedures for all sample preparation and analytical methods, giving specifics of instrumentation and procedure details, are available separately as a series of standard operating procedures.

Soil sample reception and logging

All samples from the field are transported to regional laboratories for processing. Samples collected within the AfSIS project have field descriptors in electronic format already entered in the AfSIS database. Every sample received is assigned a unique sample serial number (SSN) and is logged into

the database. Detailed procedures are given in the AfSIS Standard Operating Procedure for Sample Processing at Regional Laboratories.

Soil sample processing

Soil samples are air-dried and crushed to pass a 2-mm sieve. The total sample weight and the weight of the soil fines (<2 mm) are recorded, so that the percentage weight of the coarse fraction (>2 mm) is also known. The proportion of soil fines is a soil quality attribute in its own right. The total sample weight and weight of soil fines are also used to calculate cumulative soil mass for the augered profiles for carbon and nutrient content determination.

Soil fines are subsampled using coning and quartering (see below) or a sample divider (riffle box) to give about 350 g of soil, which is stored in a strong paper bag. Subsampling is repeated to obtain a representative 20 g subsample for shipping to ICRAF Nairobi for analysis by mid-infrared diffuse reflec-

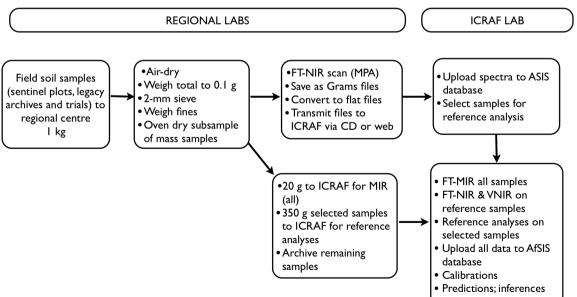


Figure 11. Schema for AfSIS soil processing.

tance spectroscopy (MIR) and other specialized analyses. Coarse fractions (20 g) are also subsampled and shipped to Nairobi for total element analysis.

The overall schema for soil sample processing is shown in Figure 11 In addition to the 20 g subsamples, selected samples of 350 g of soil fines are shipped to ICRAF-Nairobi for reference analyses. Sample selection is based on spatial stratification within sentinel sites (32 samples per sientinel site) and spectral diversity within sentinel site. Detailed procedures, including shipping procedures are given in the AfSIS Standard Operating Procedure for Sample Processing at Regional Laboratories.

3.2 Infrared spectroscopy (IR)

Diffuse reflectance infrared spectroscopy (IR) is an established technology for rapid, non-destructive characterization of the composition of materials based on the interaction of electromagnetic energy with matter.

IR is now routinely used for analyses of a wide range of materials in laboratory and process control applications in agriculture, food and feed technology, geology and biomedicine (Shepherd and Walsh, 2007). Both the visible near infrared (VNIR, 0.35-2.5 $\mu m)$ and mid infrared (MIR, 2.5-25 $\mu m)$ wavelength regions have been investigated for non-destructive analyses of soils and can potentially be usefully applied to predict a number of important soil properties determine the capacity of soils to perform various production, environmental and engineering functions (Shepherd and Walsh, 2004).

The reason that IR is useful for soil characterization is that when light interacts with a soil sample, it is absorbed to different degrees in each waveband due to electronic transitions of atoms and vibrational stretching and bending of structural groups of atoms that form molecules and crystals. In the



Figure 12. Fourier-transform near infrared spectrometer (Multipurpose Analyszr).

visible $(0.4-0.7~\mu m)$ range these differences are discernible as changes in soil colour (Bigham and Ciolkosz, 1993). Beyond the differences in colour, fundamental absorptions in reflectance spectra occur at energy levels that allow molecules to rise to higher vibrational states.

For example, the fundamental features related to various components of soil organic matter (e.g. symmetric C–H stretching) generally occur in the mid infrared range (2.5 to 25 μm ; or 4000 to 400 cm-1). Mid infrared spectra can be divided into four regions (Figure 13). Soil organic matter produces broad absorption features near 3400, 1600 and 1400 cm⁻¹, and gives rise to features throughout the spectra associated with aromatic structures, alkyls, carbohydrates, carboxylic acid, cellulose, lignin, C=C skeletal structures, ketones, and phenolics (e.g. Madari et al., 2006; Janik et al., 2007).

Clay minerals produce strong absorbance in the 3600 to 3800 cm⁻¹ region, due to hydroxyl stretching vibrations. Carbonates produce absorption with

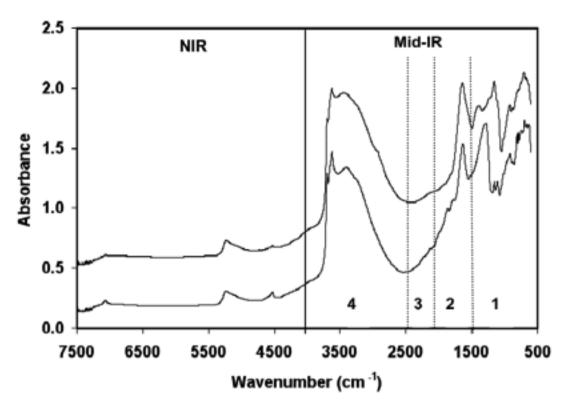


Figure 13. Soil infrared spectra: (1) fingerprint (e.g. O-Si-O stretching and bending (2) double-bond (e.g. C=O, C=C, C=N), (3) triple bond (e.g. C C, C N), and (4) X-H stretching (e.g. O-H stretching). The three main absorption features in the NIR range are principally associated with clay lattice and water OH, whereas organic matter affects the overall position and shape of the spectrum.

little interference from other minerals at 2600 to 2500 cm⁻¹ (Nguyen et al., 1991). Silica O-Si-O stretching and bending fundamentals occur in the fingerprint region (Figure 13) and their overtone/ combination bands at 2000-1650 cm⁻¹ are useful for quantitative evaluation of quartz, as the overtones are less influenced by particle size than the fundamental features (Nguyen et al., 1991).

Overtones (at one half, one third, one fourth, etc) of the frequencies of fundamental absorptions occur in the near infrared range above $4,000 \text{ cm}-1 (0.7-2.5 \mu m)$ (Figure 14). Distinctive OH^- overtone

and combination mode absorptions occur near 1.4 μm and 1.9 μm and can be used to derive estimates of soil water content as well as assessments of its degree of association with solid soil phase (e.g. Ben-Dor, 2008). Secondary (i.e. clay) minerals often have highly diagnostic spectral signatures in the VNIR region because of strong absorption of the overtones of SO_4^{2-} , CO_3^{2-} as well as OH^- and combinations of fundamental features of, for example, H_2O and CO_3^{2-} . Absorptions due to charge transfer and crystal field effects in Fe^{2+} and Fe^{3+} are particularly evident at 0.35 to 1.0 μm (Figure 14).

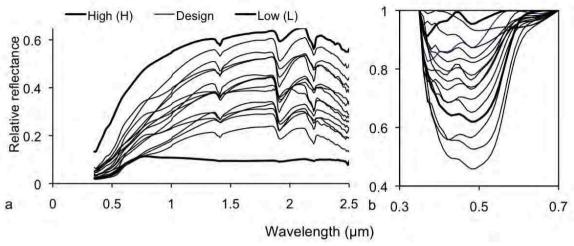


Figure 14. Diffuse visible near infrared reflectance spectra from the World Agroforestry Centre's Africa soils library. (A). Spectral selected closest to central composite design points from the principal component space plus the spectrum with the highest and lowest albedo. (B). The visible part of the same spectra shown continuum removed to emphasize the absorption features. Source: Shepherd and Walsh (2002).

In addition to the various chemical absorptions, physical properties of soils such as aggregate and particle-size distributions also affect the shape of the spectra. For pure substances the associated scattering/absorption processes are described concisely by Beer's law and the Fresnel equation.

Particle size differences are generally expected to change the baseline height of a reflectance curve without substantially altering the position of specific diagnostic features, and theoretically substances with larger grain (or aggregate) sizes have greater internal scattering path lengths from which photons may be absorbed. This would generally lower their overall reflectance baselines in the VNIR spectral region. However, in soils purely physically induced scattering processes often interact with differences in chemical composition.

For example, certain soil aggregate size classes may be associated with different quantities of organic matter, which may in turn be related to different stages of decomposition and age. Different soil particle size classes are also often associated with materials of different mineralogical origins and can have distinctively different spectral signatures. Clearly there is the potential for many other such physicochemical interactions in soils.

As a result, VNIR spectra of soils have few distinct absorption features, rendering definitive band assignments and feature-based interpretations, common in analytical chemistry and geological applications, of rather limited value. Soil spectra are therefore often difficult to interpret without resorting to multivariate pattern recognition techniques.

While this is fairly standard spectroscopic practice, a limitation of soil infrared spectroscopy is that it is largely empirical and can therefore be vulnerable to performance failures when predictions are made for samples outside the population of soils used for calibration (e.g. Brown et al., 2006).

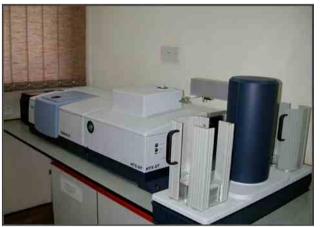




Figure 15. Left: Mid-infrared Fourier Transform Spectrometer fitted with a high-throughput screening accessory and robot for automatic loading of microplates. Right: Loaded microplate with empty wells for reference readings.

Near infrared spectroscopy in regional laboratories

Near infrared diffuse reflectance (NIR) analysis is the primary soil characterization and screening tool in AfSIS. All samples are characterized using NIR. The near infrared spectral laboratories are equipped with Bruker Fourier-Transform MultiPurpose Analyzer spectrometers (MPA) (manufactured by



Figure 16. Manually operated mid-infrared Fourier transform spectrometer.

Bruker Optik GmbH, Germany) (Figure 12).

This type of instrument was chosen for the spectral laboratory network because of their high level of reproducibility among instruments, good stability over time and temperature fluctuations, internal validation procedures, and versatility in being able to analyze a wide range of agricultural inputs and products (described in Shepherd and Walsh, 2007). Some laboratories are in addition equipped with field portable visible near infrared spectrometers (Analytical Spectral Devices), which are diffusive spectrometers (e.g. Shepherd and Walsh, 2002), which also provide versatility, but rely on external reference materials and lack internal validation routines. Samples are analyzed on both types of spectrometers where possible to provide inter-instrument calibration transfer algorithms. Details of all spectral measurements are available as standard operating procedures.

Mid infrared spectroscopy

In addition to NIR analysis, mid infrared diffuse reflectance spectroscopy (MIR) is a key soil characterization and screening tool in AfSIS. MIR has

theoretical advantages over near infrared spectroscopy for soil analysis in that light absorption due to fundamental features, as opposed to their overtones, is measured and MIR is sensitive to quartz, a key constituent of soils (Janik et al., 1988; Shepherd and Walsh, 2004). MIR also has advantages for characterization of organic matter pools (Janik et al. 2007).

However, MIR is more technically demanding than NIR and at this stage MIR measurements are centralized at ICRAF's Soil-Plant Spectral Diagnostics Laboratory. The laboratory has developed a high throughput system that does not require gas purging (Figure 15). The instrument used is a Bruker Tensor 27 Fourier-Transform spectrometer attached to a High-Throughput Screening (HTS-XT) accessory. The instrument has in-built validation procedures to guard against instrument drift.

Samples are fine ground and loaded into microtiter plates. Only a few milligrams of sample are required. A robotic arm is used for automated high throughput analysis. All AfSIS soil samples are to be characterized using high throughput MIR.

In addition all reference samples are characterized *Table 1*. AfSIS chemical soil fertility reference analysis

Analysis	Method
Organic C and N	Combustion, acidified and non-acidified
pH, electrical conductivity (EC) Exchangeable acidity	Electrodes using 1:2 volume water extract KCl extraction, unbuffered
Extractable Al, Ca, Mg, P, K, Na, S, Fe, Mn, Zn, Cu, B, Mo, H,	ICP analysis of Mehlich 3
other bases	
P sorption capacity	P Sorption Index measured by single-point P addition.

using a new manually-operated FT-MIR spectrometer (Bruker Alpha) fitted with a diffuse reflectance accessory (Figure 16). This is a low cost instrument with only an A-4 sized footprint and can be run off a battery pack. Instrument and measurement details are available in instrument-specific standard operating procedures.

3.3 Reference measurements

Organic matter

Soil organic carbon is a key indicator of soil health, providing important biological, physical and chemical functions, not least ecosystem resilience (Baldock and Nelson, 2000). Organic matter of a soil is an integral part of a soil's stock of nutrient, and its turnover both supplies nutrients and may be limited by particular deficiencies. However critical and saturation values are not yet well defined and depend on soil particle size distribution and clay mineralogy (Sanchez et al., 2003). AfSIS will develop local and global reference values for organic carbon levels for Sub-Saharan Africa.

Total and organic C and total N are analyzed at ICRAF by thermal oxidation (Skjemstad and Baldock, 2008) using a carbon analyzer according to Standard ISO 10694: Soil quality - Determination of organic and total carbon after dry combustion (elementary analysis). The instrument is a Thermoquest FlashEA 1112 including an autoanalyser. Total C and N is determined on unacidified samples and organic C on acidified samples, i.e. fumigated with hydrochloric acid to remove inorganic carbon (carbonate) (modified form Harris et al., 2001). Inorganic C is estimated as the difference between unacidified and acidified C. Soil carbon contents are determined using cumulative soil mass data obtained from weights of soil auger samples.

A carbon fraction module is proposed to determine carbon fractions, including particulate organic matter and charcoal carbon (Janik et al. 2007). Calibration of these pools to infrared spectra provides a valuable basis for soil carbon modelling (e.g. Parton et al., 1988; Zimmerman et al., 2007). These analyses will be conducted on subsets of samples in specialized laboratories.

The impacts of historic land use on soil organic carbon can be quantified using stable carbon isotopes (Boutton et al., 1998; Vågen et al., 2006a; Awiti et al., 2008), namely the relative ratio of the heavy isotope $^{13}\mathrm{C}$ to the light isotope $^{12}\mathrm{C}$ in a sample, relative to the Vienna-Pee Dee Belemnite (PBD) limestone standard. In C $_3$ plants CO $_2$ is reduced to a three-carbon compound and they generally exhibit $^{13}\mathrm{C}$ organic values in the range of – 32 to – 20 ‰, with a mean of -27 ‰ for woody plants. C $_4$ plants, however, reduce CO $_2$ to a four-carbon compound and show $^{13}\mathrm{C}$ values ranging from -17 to -9 ‰, with a mean of -14 ‰.

Stable carbon isotopes can also be used to determine the SOM turnover rates at local scales (Balesdent and Mariotti 1996, Bernoux et al. 1998), identify vegetative sources of organic matter to the soil (Roscoe et al. 2001, Krull et al. 2007), and address the impact of land conversion on soil condition (Vagen et al. 2006, Awiti et al. 2008, Schulp and Veldkamp 2008).

A natural ¹³C abundance module is analyzed on a subset of AfSIS reference samples. Carbon contents are analyzed on acidified samples by dry combustion in a C-analyzer. Natural C organic abundance is determined with an elemental analyzer coupled with an isotope ratio mass spectrometer (EA-IRMS). ¹⁵N total is also determined using the same approach on unacidified samples. Samples are analyzed in a certified isotopic analytical laboratory.

Basic chemical soil fertility

The AfSIS approach to soil fertility evaluation accommodates two paradigms of soil fertility management. The first paradigm is built around the concept of critical limits or sufficiency levels of individual constraints or nutrients in the soil, below which crops are likely to respond to added fertilizer or ameliorant, and above which they likely will not respond (Eckert, 1987, Sims, 2000).

These principles are also applied in tropical soil fertility management (Sanchez, 1976) and in the Fertility Capability Classification (FCC) (Sanchez et al. 2003) to identify inherent soil constraints and chemical limitations to soil fertility. FCC does not deal with soil attributes that can change in less than one year, but those that are either dynamic at time scales of years or decades with management, as well as inherent ones that do not change in less than a century. FCC modifiers for soil reaction include criteria for sulphidic soils, aluminium toxicity, basic reaction, alkalinity, and salinity. The FCC system does not include routine soil tests used for N and P fertilizer recommendations.

However, AfSIS measurements provide relevant modifiers for all three major nutrients, N, P and K, at Category 2, "slow, management-sensitive". The availability of N at this time scale is assessed through soil organic C measurements since C:N ratio of soil organic matter varies between relatively narrow limits around 10:1 in agricultural soils.

There are mineralogical modifiers (low nutrient capital reserves modifiers) for K, reflecting the fact that K availability is often determined by a moderately slowly available "fixed" pool. Stocks of soil P are divided between soil organic matter (assessed by soil organic C), sparingly soluble minerals and inorganically sorbed components. Availability of the latter is determined by phosphate sorption characteristics of soil Fe and Al oxides and amorphous

volcanic minerals, which often limit P availability in tropical soils. These are directly assessed with a P sorption index (PSI).

The second paradigm is based on cation nutrient balancing, which is the practice of adjusting the relative balance of levels of Ca, Mg, K, Na and exchangeable acidity in the soil, relative to the total cation exchange capacity. These concepts are based on work by soil testing laboratories (Eckert, 1987) and workers such as Albrecht and Smith (1941) and Bear and Toth (1948) in the USA, and related systems are used in Australia by Mikhail (Kinsey and Walters, 1993).

Soil testing services in eastern Africa and South Africa are also using the approach (J. Cordingley, Pers. Comm.). Ca:Mg ratios are also used to guide fertilizer recommendations in the USA and Australia (Eckert, 1987; Hazleton and Murphy, 2007). A key difference between the two paradigms, is that in the critical limits/FCC paradigm, liming would be recommended with the objective to remove Al toxicity constraints, whereas in a cation balancing system, liming aims to restore Ca levels to target levels as a percentage of cation exchange capacity. Adjusting the cation balance is claimed to promote good soil structure, optimize availability of micronutrients, stimulate microbial activity, reduce root diseases, and increase N use efficiency.



Figure 17. Laser diffraction particle size analyzer.

The cation balance system also differs from temperate agriculture approaches where liming is adjusted to bring pH values to prescribed target values. The scientific base for the cation balance approach is less well established than the sufficiency level approach (e.g. McLean et al., 1983; Kopittke and Menzies, 2007) and is likely to be less economically favorable for smallholder agricultural settings.

However, long-term benefits of this approach have still yet to be evaluated. AfSIS diagnostic agronomic trials will test the value of cation balance approaches in sub-Saharan Africa along with the development of a holistic approach to integrated soil fertility management (Vanlauwe et al., 2009).

For example, large removals of basic cations in crop produce and nitrate leaching may cause acidification under cropping if not compensated by application of basic cations in lime or organic manures (Fenton and Helyar, 2007). If the main source of fertility input is poor quality organic resources, low in basic cations, then cation depletion and acidification may result (Pocknee and Sumner, 1997).

Advisory services in the US are advocating a nutrient sufficiency approach (feed-the-crop) for short-term land tenure situations and a build and maintain approach (feed-the-soil) for longer term land tenure situations where land holders have the ability to make the longer-term investments (Mengl, 2010). The concepts are now being applied to P and K management. The feed-the-soil approach requires less frequent soil and plant testing, is less sensitive to soil test errors, and reduces risk of yield loss. However, it is not recommended in soils that are not able to retain nutrients over the longterm (e.g. sandy soils prone to leaching), and has been more widely adopted in wetter areas of the US where yield potentials are higher and risk of drought is lower.

The AfSIS basic soil chemical fertility module is designed to provide information needed to support

both of the above soil fertility paradigms (Table 1). The Mehlich 3 extraction method (Mehlich, 1984; Ziadi and Sen Tran, 2008) is used as it allows multiple elements to be analysed from one extractant using inductively-coupled plasma spectroscopy (ICP). Mehlich 3 (M-3) soil test levels also correlate well with other commonly used methods that use different extractants (e.g. Bray P-1, ammonium acetate). M-3 P has also shown to perform well in both alkaline and acidic soils across a broad range of soil types, despite the possibility of soluble P being precipitated by CaF,, a product of the reaction between NH₄F and CaCO₂ (Kleinman and Sharpley, 2002). Calibrations to Olsen P and Bray 1 and Bray 2 will be provided on reference sets to aid comparisons between alternative soil P tests. However, exchangeable acidity in AfSIS, is determined by unbuffered KCl extraction so that effective values at natural soil pH are acquired.

Extractable nutrients in soil water extracts are also determined using total X-ray fluoresence spectroscopy (see below). If this method proves successful it may replace acid extraction procedures in the future.

The sorption of phosphate (P) is an important factor controlling the fate and effectiveness of P added to soil from mineral and organic fertilizers. The P buffer capacity is the particular soil property that determines (i) the mobility and thus availability to roots of P in the soil solution and (ii) the amount of fertilizer P required to increase the soil solution P concentration. It is calculated from the gradient of the P sorption isotherm of a soil. Researchers have normally measured P sorption isotherms describing a wide range of soil solution P concentrations to obtain the P sorption capacity and P buffer capacity. However, this is too time consuming and expensive for advisory use. Bache and Williams (1971) proposed a single-point "P sorption index" (PSI) of soil that is calculated from the P remaining in solution after addition of only one P concentration. It has been found to be correlated well with the P buffer

capacity. A review of global literature has shown that this PSI, along with closely related variations, has been widely useful as a quick means of assessing P sorption across different soil types, pH values and with fertilizer P sources of both high and low solubility and mineral and organic origins. Substantial Australian research on their often very P deficient soils has established an Australian national standard PSI known as the P buffering index (Burkitt et al. 2002). A major research group in the USA has recommended a PSI method (Sims 2009) that is close to the original one of Bache and Williams (1971). American work has also shown that the extent to which soil P sorption sites are filled (Psat) is a good indicator of P availability to runoff and leachate and can be correlated with Mehlich 3 data (extractable P, Al, Fe, Ca) (Kleinman and Sharpley, 2002).

Based on a review, a PSI has been formulated for AfSIS. It needs to cope with the very wide range of soils found across Africa. In Africa, P deficiency much more of a problem than excess, and Allen et al. (2001) found that directly measured PSI was better correlated with P buffering than indirect measures. Therefore, a directly measured PSI is considered preferable to estimation of PSI or Psat from other data. The method recommended is similar that of Sims (2009). The value of the result depends on the method of P analysis (ICP or colorimetric), time and temperature of equilibration. Time and temperature of 20 hours and 25C respectively are proposed, but they may be adjusted to suit the laboratory facilities and conditions, and the chosen conditions then adhered to throughout the project.

Basic soil physical properties

The basic soil physical properties module in AfSIS includes dispersed and non-dispersed soil particle size analysis, soil moisture release curves and volume weight. Engineering properties are treated in a

separate section. Physical measurements on undisturbed samples are also treated separately. Hydraulic properties are determined through field infiltration tests.

Particle size analysis - dispersed and non-dispersed

Soil particle size distribution is a fundamental soil property that affects many soil functional properties, but its determination using conventional hydrometer or pipette methods suffers problems of poor repeatability and reproducibility and variable dispersion in many tropical soils, due to cementing actions of iron and aluminium hydroxides.

There is uncertainty on what methods best reflect functional aspects of soil particle size distribution (e.g. dispersing aggregates using dispersion agents may not reflect functional effects in the field). In fact soil particle size is usually not interpreted directly to provide information on soil functions but is rather a covariate used in predicting or conditioning soil functional properties, such as nutrient retention, tillage properties, and hydraulic properties. Therefore emphasis should be on rapid and repeatable measures rather than accurate measures of particle size distribution.

Dry aggregate size distribution has been used as an indicator of soil erodibility but it is sensitive to weather and short-term land management (Leys et al., 2002). Potential erodibility as assessed by dispersed and non-dispersed particle size distribution is a better candidate 'slow' index of soil condition (e.g. Ahmed, 1997). These indicators may have value in diagnosing soils that are susceptible to erosion, even though erodibility may be affected by a number of fast variables (e.g. Bryan, 2000).

Various measures of dispersion have been used (e.g. Emerson dispersion test, clay dispersion) to classify soil susceptibility to structural faults and piping in subsoil's (e.g. dam walls), surface soil structural

problems (e.g. hardsetting) and as an erodibility index. In AfSIS, a procedure for determining both dispersed and non-dispersed particle size distribution is used to index potential erodibility and susceptibility to erosion. This procedure measures micro-aggregate (<0.25 mm) stability, which is a slow variable, less sensitive to management than macro-aggregate (>0.25 mm) stability. Response of particle size distribution to different levels of ultrasonic energy can be used to derive an absolute measure of soil stability (North, 1976).

All particle size analysis methods have limitations and different methods give different results. To provide rapid and repeatable comparative estimates of particle size distribution, with the objective to provide estimates of functional attributes of particle size distribution among AfSIS samples, laser diffraction particle size analysis is used. This is a relatively new technique (e.g. Gee and Or, 2002; Ariaga et al. 2006) but has high levels of repeatability and can be done using small quantities of soil (<5 g). A representative cloud or 'ensemble' of particles passes through a broadened beam of laser light which scatters the incident light onto a Fourier lens. This lens focuses the scattered light onto a detector array and, using an inversion algorithm, a particle size distribution is inferred from the collected diffracted light data. Mie theory is used to provide a volume-based continuous distribution of particle sizes based on the correlation between the intensity and the angle of light scattered from particles (Xu, 2000).

AfSIS samples are analyzed using a Horiba Model LA 950A2 with a detectable size range of 0.01-3000 microns (Figure 17). The instrument allows continuous flow of a suspended soil sample, to which different sonification cycles can be applied using an in-built ultrasonic probe. The protocol (under development) begins with measurement of particle size distribution in dry soil suspended in an air stream to provide a measure of microaggregation without wetting. Particle size distribution is then

measured over time in water, followed by sonification cucles, and finally full dispersion using Calgon. The shift in particle size distribution with these treatments is used to provide comparative indices of stability (e.g. Muggler et al, 1996). Effects of mechanical and chemical dispersion forces can be assessed separately. Destruction of organic matter and removal of soluble, salts, gypsum, carbonates, and iron and aluminium oxides is not be done with this method, as comparisons of 'functional' particle size distribution is of primary interest, as opposed to accurate measurement of 'absolute' particle size distribution of primary particles. A subset of soils

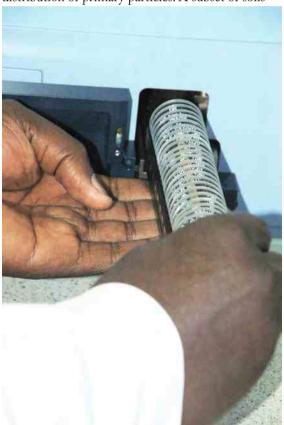


Figure 19. Loading samples on tray into total x-ray fluorescence spectrometer.



Figure 18. Total x-ray fluorescence spectrometer.

is also analysed using the conventional hydrometer method to provide correlations with the laser diffraction measurements.

When sampling permits taking of undisturbed or semi-disturbed samples, a modified Emerson dispersion test (Field et al., 1997) is done for comparison with the laser diffraction results.

Soil moisture release curves

Soil moisture release curves express the relationship between matric potential and water content in soil. The shape and position of the curve determine hydraulic properties, such as infiltration rate, plant available water holding capacity, and aeration. Matric potential is expressed here in units of work per unit weight (m water at 20 C; dimensions L), as this unit is easy to visualize (Cresswell and Hamilton, 2002).

Intact soil cores are required to provide data that is representative of field macrostructure conditions for the range 0 to -30 m potential, but soil fines are best for potentials -30 to -150 m. Due to the difficulty of taking and transporting intact soil cores, AfSIS has two sub-modules for soil moisture release curves. Soil fines are used for the standard sentinel site reference samples, and intact cores, taken from soil

pits, are used where feasible.

For AfSIS reference samples, soil moisture release curves are determined using soil fines in pressure plate apparatus (Cresswell and Hamilton, 2002; Dane and Hopmans, 2002). The procedure is modified to use repeated measurements at different potentials on small (2 cm diameter) reconstructed cores. A standard weight of soil fines is poured into the cores, without firming. Bulk density is measured using a calibrated volumetric scoop. Cores are sealed off at the bottom using fine muslin cloth taped to the core. Soil moisture content is determined at three potentials only: saturation, -1.0 m and -150 m. The two-point method of Cresswell and Paydar (1996) is used to estimate the soil moisture characteristic using the Hutson and Cass (1987) modification of the Campbell equation, a continuous two-piece function suitable for use in soil water simulation models (McKenzie and Cresswell, 2002).

Intact cores are not sampled as part of the standard sentinel site protocol, and generally required soil pits to be dug to obtain good quality samples from diverse soil types. However where a field sampling module for obtaining undisturbed cores can be implemented, full soil moisture release curves using pressure plates are done (Cresswell and Hamilton, 2002).



Figure 20. Benchtop x-ray diffraction spectrometer.

Volume weight

Volume weight is the weight of a known volume of soil fines at a specified water content. Values give an indication of soil physical condition and allows conversion of test results to volume units. Volume weight is determined by weighing a scoop of soil of known volume dried to a standard moisture content.

Element profiling

AfSIS extends soil fingerprinting concepts developed using infrared spectroscopy (Shepherd and Walsh, 2007) into the X-ray range using soil total element profiles. All soils contain some of all of the naturally occurring chemical elements. Variation in the concentration of elements is derived from differences in the composition of the parent material and from fluxes of matter and energy into or from soils over geologic time (Helmke, 2000). Hence element profiles (Kabata-Pendias and Mukherjee, 2007) are a marker of differences in soil forming factors and may therefore form a useful basis for classifying soils in a way that relates to inherent soil functional properties.

For example, Rawlins et al. (2009) recently demonstrated use of element profiling for the prediction of particle size distribution. Analysis of refractory element concentrations have also been used in element mass balance estimation (Chaddwick et al., 1999; Kutz et al., 2000). Total elemental ratios can be used to indicate degree of soil development and rates of weathering (Birkeland, 1999), as well as provide information on the soils' maximum nutrient capacity.

In AfSIS, multivariate analysis of element profiles is used as a covariate, in conjunction with infrared spectroscopy, to predict soil functional properties. Element determinations are also used to assess micronutrient deficiencies and heavy metal pollution. Emphasis is placed on identification of syndromes,

not only individual nutrient constraints. For example, micronutrient deficiencies tend to occur in sandy soils with low organic matter content, and this syndrome can be diagnosed spectrally. Furthermore, interventions often need to be targeted at the syndromes and not individual nutrient deficiencies (e.g. build up organic matter to supply missing nutrients, increase nutrient retention capacity and improve soil structure).

Micronutrients

Micronutrients, or trace elements, are chemical elements that are needed in minute quantities for the proper growth, development, and physiology of plants, animals or humans (Bowen, 1976). A deficiency of one or more of the eight plant micronutrients will adversely affect both the yield and quality of crops. These are: boron (B), chlorine (Cl), copper (Cu), iron (Fe), manganese (Mn), molybdenum (Mo), nickel (Ni), and zinc (Zn). Animals need all of these elements as well as chromium (Cr), cobalt (Co), fluorine (F), iodine (I), selenium (Se), silicon (Si), sodium (Na), and vanadium (V).

Major human micronutrient deficiencies include Fe, I, Se, Zn, and various vitamin deficiencies. Se and Co, although not required by plants, may be enough to satisfy human requirements fully in fertile soils; however, probably half of all soils are deficient in at least one of the ultra-micronutrients Se, I or Co.

Fortification of commercially available staple foods is not a solution to malnutrition in subsistence farming sectors, and there is need to identify, assess and correct soil micronutrient deficiencies for sustainable agricultural systems and improved human health. In particular there is opportunity for fertilizer strategies to have significant impacts on Zn, Se, and I deficiencies in humans. Cobalt fertilizer may need to be used in some subsistence food systems where soil-available Co is low because Co is

a constituent of vitamin B12.

Bioavailability of micronutrients is determined principally by soil mineralogy, organic matter, pH, and redox reactions (Mortvedt, 2000). AfSIS focuses on quantifying the risk factors associated with micronutrient deficiency syndromes as a basis for rapid diagnostic tests using spectral inference methods. Micronutrients are determined in soil and soil water extracts on AfSIS reference samples. Micronutrients are also measured in tissue and grain samples from AfSIS agronomic trials.

Heavy metals

Bowen (1979) has suggested that when the rate of mining of a given element exceeds the natural rate of its cycling by a factor of ten or more, the element should be considered a potential pollutant. Thus the most hazardous trace elements to the biosphere may be: Ag, Au, Cd, Hg, Pb, Sb, Sn, Te, and W. Also those elements that are essential to plants and humans, such as Cr, Cu, Mn and Zn, may be released in excessive amounts in some regions (Kabata-Pendias and Mukherjee, 2007).

Soil quality standards for heavy metals are often based on the total soil heavy metal concentration extracted by strong acid destruction. In many cases, differences in soil type or soil properties (acidity, clay and organic matter concentration) are included only marginally, if at all. However, the degree to which heavy metals are available to plants or soil organisms, or leach to the groundwater largely depends on a combination of these soil properties and the source of the metals in the soil. For agriculture, one of the key aspects is safe food production, apart from groundwater protection and ecological aspects. Multiple regression of concentrations of heavy metals in crops against their concentrations in soil plus other soil covariates, such as pH, clay, and organic matter levels is a promising method for setting probablistic standards (Brus et al., 2005). Heavy metals are determined in soil and soil water extracts on AfSIS reference samples. Heavy metals are also measured in tissue and grain samples from AfSIS agronomic trials.

Analytical method

AfSIS employs high throughput Total X-Ray Fluorescence Spectroscopy (TXRF) (Figure 19). This relatively new technique (KlocKenKämper, 1997) provides for rapid simultaneous analysis of all elements from Na to U (except Mo) with minimal sample preparation time. The main principle of X-ray Fluorescence Spectroscopy is that atoms, when irradiated with X-rays, emit secondary X-rays – the fluorescence radiation.

On this basis XRF analysis is possible because (i) the wavelength and energy of the fluorescence radiation is specific for each element, and (ii) the concentration of each element can be calculated using the intensity of the fluorescence radiation. Standardization is internal and only requires addition of an element that is not present in the sample for quantification purposes, and no external standardization is required in most cases.

A monochromatic X-ray beam is directed onto the sample at a very small angle ($< 0.1^{\circ}$) causing total reflection of the beam. The characteristic fluorescence radiation emitted by the sample is detected by an energy-dispersive detector and the intensity is measured by means of an amplifier coupled to a multichannel analyzer.

The main difference with respect to common XRF spectrometers is the use of monochromatic radiation and the total reflection optics. Illuminating the sample with a totally reflected beam reduces the absorption as well as the scattering of the beam in the sample matrix. Resulting benefits are a greatly reduced background noise, and consequently much

higher sensitivities and a significant reduction of matrix effects. Another major advantage of TXRF, compared to atomic spectroscopy methods like AAS or ICP-OES, is the avoidance of memory effects.

Powders are prepared directly or as a suspension, and liquids are pipetted directly onto sample carriers. Only small samples of 20 –50 mg of soil are required and minimal sample amounts can be in the low μg / μL range. The Lower Limits of Detection (LLD) for many elements is close to or below 1 μg /l.

AfSIS samples are analyzed using a Bruker Picofox TXRF instrument at the ICRAF Soil-Plant Spectral Diagnostics Laboratory. Soils are ground to <50 μm and prepared as suspensions. Sample analysis time is about 10 minutes. A protocol for element profiling of soil water extracts is in preparation to estimate element availability to plants.

3.4 Mineral profiling

Despite the critical importance of soil mineralogy in the determination of soil functional properties and as a soil forming factor (Jenny, 1941), there has been relatively little work to move beyond largely descriptive studies (Dixon and Weed, 1989; Dixon and Schulze, 2002) to the quantitative linking of soil function to soil mineralogy (Cornu et al., 2009; Andrist-Rangel et al., 2006). New instrumentation developments in bench top high-throughput X-ray powder diffraction spectroscopy (XRPD) and steady improvements in mineral identification databases and software have opened up new opportunities for quantitative determination of mineral phases on large sample numbers. AfSIS extends the infrared spectroscopy profiling approach (Shepherd and Walsh, 2007) to include X-ray diffraction spectroscopy. X-ray diffractograms are directly input to pedotransfer functions and mineral phase identifica-

Functional soil properties and their inference from reference properties Table 2.

Functional property	Inference method	Measured 'reference' properties			
Soil physical properties					
Texture type (FCC) in topsoil and subsoil	Texture type calibrated to spectra Organic carbon calibrated to spectra	Particle size distribution; depth restrictions from field data for R substrata type; soil organic carbon in top 50 cm for organic soil (O) type.			
Waterlogging modifier (FCC)	-	Field data.			
Strong dry season modifier (FCC)		Climatic data layer.			
Low soil temperatures modifier (FCC)	-	Climatic data layer.			
Gravel modifier (FCC)	Coarse fraction weight	Coarse fraction as percentage weight of total sample.			
Slope modifier	-	Field data			
High erosion risk modifier (FCC)	 Class direct from PSD Class calibrated to spectral discontinuity 	Particle size distribution (PSD). Soil depth and slope from field data.			
Soil moisture release curve; upper and lower limits of plant available water; available water holding capacity	Mositure release curve parameters calibrated to spectra PTF-estimated moisture release curve parameters calibrated to spectra	Moisture release curve; particle size distribution, organic C, bulk density.			
Erodibility; hardsetting/crusting risk	Class calibrated to spectra	Dispersed vs non-dispersed particle size distribution; soil organic C; Mehlich 3 Na; XRPD data.			
Saturated hydraulic properties	Infiltration curve parameters calibrated to topsoil and subsoil spectra	Field measured inflitration curves.			
Unsaturated hydraulic properties	PTF-estimated hydraulic parameters calibrated to spectra	Particle size distribution, organic C, bulk density; XRPD data.			
Engineering properties (plasticity index, liquid limit; tunelling/piping; leaking; slumping; cracking; optimum moisture content; USCS class)	Classes calibrated to spectra	Particle size distribution (dispersed vs non-dispersed); plastic and liquid limits; coarse fraction; organic C; XRPD data.			

Table 2 cont.

Functional property	Inference method	Measured 'reference' properties				
Soil chemical properties						
Soil organic carbon and nitrogen pools	Pool size calibrated to spectra	Total C, organic C and N, particulate organic C, charcoal C				
Sulfidic modifier (FCC)	Class calibrated to spectra	pH				
Aluminium toxicity for most crops modifier (FCC)	Class calibrated to spectra	pH, Exch. Acidity; Mehlich 3 Al.				
No major chemical limitations modifier (FCC)	Class calibrated to spectra	Exch. Acidity; Mehlich 3 Al.				
Calcareous modifier (FCC)	Class calibrated to spectra	Inorganic C, pH				
Salinity modifier (FCC)	Class calibrated to spectra	EC, pH				
Alkalinity modifier (FCC)	Class calibrated to spectra	pH, Mehlich 3 Na				
Geological salinity risk	Class direct from XRPD	XRPD quantification of souble minerals				
Lime requirement and source type	1. Requirement calibrated to spectra	Exch. acidity; Mehlich 3 cation balance; pH; particle size distribution				
	2. Source type calibrated to spectra					
Low available P	Class calibrated to spectra	Mehlich 3 P; P sorption index; XRPD/TXRF data; particle size distribution				
Environmental P risk	Class calibrated to spectra	Mehlich 3 P; P sorption index; XRPD/TXRF data; particle size distribution				
Micronutrient deficiency	Class calibrated to spectra	Mehlich 3 micronutrients, pH; particle size distribution; soil organic C; TXRF/XRPD data.				
Heavy metal pollution	Class calibrated to spectra	TXRF soil and extracts; particle size distribution; soil organic C; pH.				
Anion retention capacity	Class calibrated to spectra	Exch. Acidity; Mehlich 3 H, A; pH; organic C; particle size distrubution; XRPD data.				
High pesticide retention/leaching risk	Class calibrated to spectra	Organic C, pH, particle size distrubution; XRPD data.				

tion and quantification are used for interpretation.

X-ray powder diffraction requires that a sample be prepared as a randomly oriented powder. For preparation of powder samples from soil fines, wet milling with water or ethanol (Methanol) is done in a Mc-

Crone micronizing mill. The mixture is then dried at $80\,^{\circ}\text{C}$ or centrifuged at high speed for $10\,\text{min}$ and decanted. Hexane is then added to the sample in the ratio of $0.5\,\text{ml}$ hexane to $1\,\text{g}$ of sample. After mixing the sample is dried at $80\,^{\circ}\text{C}$ and then sieved

Table 2 cont.

Functional property	Inference method	Measured 'reference' properties		
Soil organic carbon pools	Pool size calibrated to spectra	Total C, organic C, particulate organic C, charcoal C.		
Mineralogical properties				
Low nutrient capital reserves modifier (FCC)	Class calibrated to spectra	Mehlich 3 K, CEC; XRPD/TXRF data		
High P fixation by Fe and Al oxides modifier (FCC)	Class calibrated to spectra	P sorption index; Mehlich 3 P, Al, Ca, Fe; XRPD/TXRF data.		
Amorphous volcanic modifier (FCC)	Class calibrated to spectra	pH; XRPD data; P sorption		
Cracking clays modifier (FCC)	Class calibrated to spectra, PSD	Particle size distribution; XRPD data; Linear shrinkage		
High leaching potential modifier (FCC)	Class calibrated to spectra	Mehlich 3 cations, CEC; Particle size distribution; XRPD data.		
General soil fertility rating	Class calibrated to spectra	Mehlich 3 cations, exch. acidity, pH, particle size distribution, coarse fraction, organic C, XRPD and TXRF data.		

Biological properties					
Low organic carbon saturation	Saturation deficit calibrated	Organic C, sand; local and global reference values from AfSIS			
modifier (FCC); with Walsh &	to spectra	database based on land cover, ¹³ C.			
Vagen modification.					

through a 250 μm sieve. A fraction or portion of the randomly oriented powder is loaded into a plastic sample holder by the razor tampered method.

For more detailed analysis of clay fractions, samples are soaked with water and sonicated for 5 minutes. The mixture is transferred into a volumetric flask and left overnight to allow the coarser material to settle and the clay suspension is then siphoned into a beaker and filtered with a vacuum filter. The clay on the filter is then mounted on a glass slide and air dried.

XRPD measurements are done using a benchtop X-ray diffractometer system (Bruker D2 Phaser). The D2 Phaser is a high quality integrated XRPD system that does not require external components

(such as chiller, computer system, display) and needs only normal mains power supply. The instrument is equipped with a LYNXEYE compound silicon strip, 1-dimensional detector with Theta / Theta geometry. The angular range is -2.5 to 145° 2Theta with an accuracy of ± 0.02° throughout the measuring range. The instrument is integrated with the DIFFRACplus TOPAS graphics based, non-linear least squares profile analysis program. TXRF soil element information is also used to focus mineralogy searches.

Identification of X-ray minerals is achieved by comparing the X-ray diffraction pattern (diffractrogram) obtained from an unknown sample with an internationally recognized database (Powder diffraction file, PDF) containing reference patterns with more

than 70000 phases. Quantitative phase analysis of crystalline powder samples is done using a full pattern fitting methods (Rietveld method e.g. using TOPAS). A library of African minerals is also being established as an aid to pattern fitting methods.

3.5 Engineering properties

Soil mechanical properties are not only important for many engineering decisions (e.g. road construction, dam construction, earthworks) but also determine structural stability and tillage properties (e.g. workability) of soils.

AfSIS determines several soil engineering properties on reference samples, in addition to those determined in the basic soil physical properties module. There is a wide range of soil tests used for engineering purposes, however, a small set of tests has been selected for AfSIS, on the basis of ease of use and ability to infer many other engineering properties (Bell, 2000; Hazelton and Murphy, 2007).

These are the Atterberg consistency limits, linear shrinkage test, and hygroscopic water content. These are capacity measurements, which are constant but which differ by location (i.e. slow variables) as distinct from intensity measurements, which are dynamic with respect to internal or external conditions, and include stress/strain and soil strength (fast variables) (Horn and Baumgartl (2000).

The Atterberg consistency limits (e.g. Kirby, 2002) are the most meaningful and widely interpreted of soil engineering indices, being used to estimate the shear strength and bearing capacity, compressibility, swelling potential, and specific surface of soils. However, there are problems with the poor reproducibility of the standard methods (soil thread method for liquid limit; cone penetrometer or Casagrande method for plastic limit).

Derivation of the Atterberg limits from the soil moisture release curve has been proposed on theoretical grounds and has shown promise for Canadian soils (McBride, 1989).

The liquid limit, upper plastic limit, of a soil represents the moisture content where the primary particles or aggregates are almost completely separated by interstitial water. This point is analogous to the moisture content above which water is retained with essentially no force, or the upper flex point of the desorption curve.

Similarly, the point at which the remaining adsorbed water is in a highly rigid and structured state, or the lower flex point, should correspond with the point of maximum soil cohesion in most soils (i.e. the plastic limit or lower plastic limit). It follows that the region of the curve between these flex points represents the range of moisture content over which a soil exhibits plastic properties.

Soil shrinkage is used by engineers as an important factor determining material stability associated with building and soil conservation structures, and by agriculturalists in relation to tillage and soil physical rehabilitation. The linear shrinkage test based on the Australian Standards Association (McGarry, 2002) is used by AfSIS as it has shown to be more reproducible than several alternative tests.

Hygroscopic moisture content of the soil is associated with a number of properties such as surface area, cation exchange capacity, liquid limit, swelling potential, and electrical properties (conductivity and dielectric constant). Hygroscopic moisture is determined as the moisture content of air-dry soil, determined by oven-drying at 105 °C.

3.6 Radionuclides

Fallout radionuclides inventories of 137Cs, 210Pb

and 7Be are often used to estimate rates of soil erosion and/or deposition (soil redistribution) in landscapes (e.g. Owens and Collins, 2006). Analysis is conducted by gamma-ray spectroscopy (e.g. Baskaran et al., 1991). Analysis is slow (e.g. 24-hours per sample) and expensive and thus only restricted sets of AfSIS reference samples are analysed for ¹³⁷Cs, and ²¹⁰Pb. Analysis is done in specialized laboratories in the USA and Europe.

Airborne and ground-based gamma-ray spectroscopy is also used in geophysical survey to detect natural emission of gamma radiation from the upper 0.3-0.4 m of the land surface. Spontaneous radioactive decay of unstable isotopes in rocks and soils produces gamma radiation and radioelement profiles relate to the mineralogy and geochemistry of the soil regolith and can be used as a predictor in digital soil mapping (Wilford, 2008).

Radionuclide profiling of AfSIS soil reference samples in the laboratory by gamma ray spectroscopy is being investigated in preparation for airborne surveys, which may be feasible in Africa in the future. It is proposed to analyze samples using a Bruker laboratory HPGe spectrometer with shield. Separate and simultaneous measurement of the activity of 100 radionuclides is feasible with this technique.

3.7 Soil biological properties

Soil biological processes are essential to the production and environmental services of soils. These processes include decomposition, nutrient cycling, SOM formation and mineralization, soil aggregation, regulation of atmospheric trace gases and the biological control of soil-bourne plant and animal pests and diseases (Lavelle et al., 1994). However, soil science is still challenged to find interpretable 'slow' indicators of soil biological function and their

critical levels needed to maintain key soil processes (Sanchez et al. 2003; Abbot and Murphy, 2007). This is bourne out by the lack of soil biological indicators in soil test interpretation manuals (e.g. Landon, 1984; Brown, 1987; Peverill et al., 1999; Hazelton and Murphy, 2007; McKenzie et al. 2008).

Most methods of soil biological characterisation require fresh samples or large samples or special sample preservation techniques, such as freezedrying, and this module therefore requires an additional field sampling campaign. Analysis of airdried samples for DNA profiling is done using the procedures below. A module for soil faunal DNA profiling using fresh samples is under development.

Soil sampling and DNA isolation

The protocol for sampling soils has been outlined previously (Fierer and Jackson, 2006), however, in AfSIS the air-dried 2-mm sieved fine fraction will be used. Approximately 10–20 g of composite soil is required for analysis. Bags of air dried soil samples are shipped (preferably via DHL, UPS, FedEx, or first class mail) boxed or contained within a Styrofoam cooler, with the bags of soil secured within the container using packing material (e.g., newspaper or bubble wrap) to the micorbial laboratory for analysis. Upon receipt, the samples are archived at -80°C until DNA extraction.

For each of the composite soil samples, ~10 g of soil is removed and further homogenized under liquid N₂ using a mortar and pestle. Soil community DNA is then extracted from a 0.5 g subsample using a commercial extraction kit (PowerSoil DNA, MoBio Laboratories, Carlsbad, CA, USA). After an additional incubation step (65°C for 10 min followed by 2 min of bead beating) to optimize soil community DNA extraction and limit shearing, the manufacturer's protocol are followed. Eluted DNA is be stored at -20°C until used in PCR amplifica-

tion.

PCR-amplification of rRNA genes and bar-coded pyrosequencing

Preparation of extracted DNA for pyrosequencing follow the protocol described previously [Fierer et al., 2008; Costello et al., 2009 (see supplementary material); Lauber et al., 2009]. Briefly, the method includes targeted amplification (using group-specific primers) of a portion of the small-subunit ribosomal gene (16S for bacteria and archaea or 18S for fungi), triplicate PCR-product pooling (per sample) to mitigate reaction-level PCR-biases, and Roche 454 pyrosequencing. Forward primers include a Roche 454 A pyrosequencing adapter, while reverse primers incorporated a bar-code sequence (unique to each individual sample), a 2bp linker, and a Roche 454 B sequencing adapter.

PCR reactions are preformed in 25 µl reactions, each containing forward and reverse primers, commercial PCR master-mix kit, and genomic community DNA as a template. PCR cycling parameters are specific to individual primer sets. Pooled triplicate reactions are quantified using PicoGreen dsDNA assay (Invitrogen, Carlsbad, CA, USA). A single composite sample (representing all soil sites) is then produced that contains the bar-coded PCR product, normalized in equimolar amounts to produce consistent reads, which is then pyrosequenced on a Roche GS-FLX 454 automated pyrosequencer.

Sequence processing and assigning taxonomic identity

Prior to analyses, raw sequence data generated from the 454-sequencing runs are processed to assure quality and to assign a taxonomic identity to each of the >400,000 sequences per run. In brief, sequences are removed from the dataset which have uncorrectable bar-codes or that have low quality scores (<25),

or that are reads which are below the expected amplicon size for a given primer set. The remaining sequences are binned into phylotypes (≥ 97% similarity) using Cd-Hit (Li and Godzik, 2006) and grouped by samples according to their unique 12 bp bar-code. Phylotypes are then assigned an identity (at ≥ 60% similarity level) based on comparisons with sequences in a public database (Ribosomal Database Project; http://rdp.cme.msu.edu/) under the RDP taxonomic structure (Cole et al., 2005). A composite alignment is created using representative sequences for each phylotype identified using the NAST alignment function of the GreenGenes public database (http://greengenes.lbl.gov/) with hypervariable regions removed with a PH Lane Mask.

The sequence alignment is then used to infer phylogenic relationships between all sequences in order to calculate a community-level phylogenetic distance between each pair of samples. Sequence quality assurance, taxonomic assignment, and subsequence analyses of community structure are handled in the QIIME software package (http://qiime.sourceforge.net/).

This workflow, as well as other standard analyses for soil communities (prokaryotic and eukaryotic), have been described in previous publications [Fierer et al., 2008; Hamady et al., 2008; Costello et al., 2009 (see supplementary material); Lauber et al., 2008; 2009].

Finally, sequences representative of individual phylotypes will be deposited in the GenBank short read archive and all data related to sequences will be made available online via a publicly-accessible database.

Carbon saturation deficit

Sanchez et al. (2003) have proposed carbon saturation deficit as a biological indicator, where organic

carbon levels are compared with undisturbed or semi-natural reference sites under the same soil type. In AfSIS a modification of this approach is used by first normalizing organic carbon with sand content, recognizing the textural control on potential carbon concentrations.

3.8 Plant growth bioassay

Plant growth bioassays conducted using pot studies constitutes a useful tool to supplement field testing for diagnosis of plant nutrient deficiencies and development of soil fertility management recommendations. Plant bioassays are recommended in AfSIS for benchmarking relative productivity of soils without added ameliorant and comparative quantification across soils of responses to nutrient inputs. Procedures describe by Awiti (2006) are recommended combined with infrared spectral analysis of soil and leaf material. In addition fertiliser response trials are conducted at selected AfSIS sentinel sites.

3.9 Analyses for soil classification

A number of additional laboratory tests are required for soil classification in the Soil Taxonomy (Soil Survey Division Staff, 1993) and FAO/UNESCO (FAO-Unesco-ISRIC, 1990) systems. These analyses are performed in specialized laboratories (e.g. through ISRIC or USDA) in conjunction with a separate field campaign in this optional module.

3.10 Pedotransfer functions

AfSIS emphasizes soil functional properties that change only slowly in relation to edaphic and management factors. Pedotransfer functions are used

to predict values of soil functional properties for the entire set of sampled soils (minimum of 32,280 samples) based on the laboratory reference measurements (minimum of 1,664 samples).

Digitial soil mapping in turn relates these values to geospatial information to predict values of soil functional properties at any given geographical location. The basic form of the pedotransfer model is:

$$S = f(Q) + e$$

Where S is a soil property or condition of interest, Q is a vector of covariates (such as laboratory reflectance data) and e is an uncertainty parameter.

Several approaches to predicting and interpreting soil functional properties are used:

- Calibration of individual measured sample reference measurements to infrared spectral data.
 Other high throughput laboratory measured properties may also be included (e.g. TXRF, XRPD data) as predictors along with the spectral data. Various data reduction methods are used to reduce the dimensions of the spectral data.
- Calibration of derived or interpreted soil functional properties or classes to infrared spectral and other high throughput data. The derived properties or classes may be based on multivariate analysis of reference data (e.g. principal components or cluster analysis) or some other criterium, such as the probability of being above or below a critical limit (e.g.), composite indicators (e.g. exchangeable Ca:Mg ratio), or a soil management receommendation (e.g. lime requirement).
- Multivariate classification of soil spectral data for the entire sampled set of soils, which is then interpreted in terms of the distributions of soil reference measurements (e.g. see Vågen et al., 2006b). Multivariate analysis of soil reference

values may also be used as an interpretation guide.

Calibration of reference measurements or derived values to infrared spectral data and other georefernced covariates in spatially explicit hierarchical models. Reference measurements are directly included in digital mapping models. Usually the number of reference measurments available limits this approach, however prior stratification based on geographical variables may often be feasible.

A number of different mutlivariate calibration algorithms are tested, including partial least squares regression (e.g. Shepherd and Walsh, 2002; Terhoeven-Urselamans et al., 2009), boosted classification and regression trees (e.g. Shepherd et al., 2005; Brown et al. 2006), and support vector machines in conjunction with wavelet decomposition.

The spectral library approach outlined in Shepherd and Walsh (2002) is applied. Various spectral distance metrics are used to determine whether an unknown sample falls within the same population as the calibration samples (e.g. Naes et al., 2002; Tranter et al., 2009).

As far as possible soil functional properties are measured directly on the reference soil samples and calibrated directly to soil infrared spectra (Shepherd et al., 2002). Where soil functional properties cannot be directly measured (e.g. unsaturated hydraulic conductivity) pedotransfer functions published from the literature may be used to infer values of the functional properties from the laboratory reference data (e.g. Campbell 1985; Minansy et al., 2008). McBratney et al. (2006) proposed infering functional properties as a second step using spectrally inferred primary properties (e.g. clay, sand, organic matter).

In AfSIS, we propose direct calibration of either the measured functional properties or their inferred properties to spectral data, as proposed in the spectral library approach proposed by Shepherd and Walsh (2002; 2007), to reduce error propagation and improve model fits. Caution is advised is transferring pedotransfer functions from one population of soils to another.

3.11 Interpretation of soil tests

Currently there is no soil test interpretation guide available for African soils and so AfSIS is developing one, drawing strongly on guidelines available for tropical soils from the FCC system (Sanchez et al., 2003) and international soil survey experience (e.g. Landon, 1984), and work in Australia (e.g. Peverill et al., 1999; Hazelton and Murphy, 2007), USA (e.g. Benton Jones, 2003) and Latin America (e.g. Cochrane et al., 2005). Synthesis of Africa soils work and new agronomic testing in AfSIS will also inform this guide.

Key functional properties currently considered in AfSIS are given in Table 2, and this framework is being further developed under the project.

Spectra is defined as infrared spectral data plus optionally other types of spectral data (XRPD, TXRF, laser diffraction particle size). Pedotransfer functions (PTF) are sometimes used as an intermediate step to estimate funtional properties from reference measurements; the PTF-predicted values are then calibrated to spectra.

Table 2 places heavy reliance on definition of interpreted recommendation classes and the direct calibration of classes to spectra, although in some cases the classes may be derived retrospectively after calibration of continuous variables to spectra. Classes are drawn up based on guidelines from the literature (e.g. FCC) and expert opinion, with emphasis on tropical and sub-tropical soils.

Uncertainty in class assignment from input of either data, literature values, or expert opinion can be represented, for example in the form of Bayesian Belief Networks (e.g. Bashari et al., 2009). Such tools are becoming an increasingly popular modelling tool in ecology and environmental management because their diagramatic form aids communication (e.g. Cain et al., 2003), while using probabilities to quantify relationships between model variables, explicitly allows uncertainty and variability to be accommodated in model predictions.

This approach can be extended to include spectral data as well, if reduction to a small number of spectal dimensions is sufficient to provide adequate prediction. The functional properties or guidelines in turn can be incorporated into decision models that include other variables. Further functional capacity interpretations are added as new user needs are identified. A key output is the prevalence of different soil constraints at site and cluster levels to guide intervention strategies.

3.12 Plant analysis

Plant analysis is done to support AfSIS agronomic trials and in particular to couple plant tissue analysis with soil analysis for diagnosis of soil fertility constraints. In particular there is need to develop guidelines for limiting levels of elements and element ratios in plant tissues in African soils for major crops. In addition analysis of the composition of organic and inorganic ameliorants used in AfSIS trials is required.

There are two main types of systems used for intepreting plant analysis: the Sufficiency Range system (SR), and the Diagnosis and Recommendation Integrated System (DRIS) (Baldock and Schulte, 1996). SR considers individual elements with respect to critical limits defining ranges such

as deficient, sufficient and high. DRIS was actually developed in South Africa (Beaufils, 1973) and was adapted and advanced in the USA by Sumner (1977; 1979). DRIS uses ratios of all possible nutrient pairs compared with ratios found in high yielding crops. Baldock and Schulte (1996) combined both systems into the Plant Analysis with Standardized Scores (PASS) system.

AfSIS uses TXRF for simultaneous multielement tissue and organic resource analysis for many of the elements from Na to U, except Mo. N analysis is done using near infrared spectroscopy calibrated to combustion or Kjeldahl reference analysis (Shepherd et al. 2003). Organic resource quality classes are also derived from NIR analysis (Shepherd et al. 2003).

3.13 Definitions and abbreviations

ASD. Analytical Spectral Devices field spectrometer

BBN. Bayesian belief networks. Graphical models consisting of nodes (boxes) and links (arrows) that represent system variables and their cause-and-effect relationships. Also known as belief networks, causal nets, causal probabilistic networks, probabilistic cause effect models, and graphical probability networks.

DRIS. Diagnosis and Recommendation Integrated System for interpreting plant analysis results.

Infrared spectroscopy. Infrared spectroscopy is taken to include diffuse reflectance, transmission, transflectance and attenuated total reflectance spectroscopy within the visible (vis; $0.35~\mu m$ to $0.75~\mu m$), near infrared

- (NIR spectroscopy; $0.75~\mu m$ to $2.5~\mu m$) and mid infrared (mid-IR spectroscopy; $2.5~\mu m$ to $25~\mu m$) wavelength range.
- ISRIC. International Soil Reference Information Service.
- Laser diffraction particle size analysis. Particle size analysis based on light diffraction from particles suspsended in an air or liquid stream.
- Liquid limit. Depending on the water content of the soil, it may appear in four states: solid, semi-solid, plastic and liquid. The liquid limit is the water content where a soil changes from plastic to liquid behavior.
- LLD. Lower limit of detection. The lowest quantity of a substance that can be distinguished from the absence of that substance (a blank value) within a stated confidence limit (generally 1%).
- NIR. Near infrared diffuse reflectance spectroscopy (wavelength range 8,000 to 4,000 cm-1 or 1,250 nm to 2,500 nm).
- MIR. Mid-infrared diffuse reflectance spectroscopy (wavelength range 4,000 to 400 cm-1 or 2,500 to 25,000 nm).
- MPA. Multipurpose Analyzer. The model of the Bruker Fourier-Transform near infrared spectrometer used in the AfSIS spectral laboratory network.
- Pedotransfer function. Predictive functions of certain soil properties from other more available, easily, routinely, or cheaply measured properties.
- Plastic limit. Depending on the water content of the soil, it may appear in four states: solid, semi-solid, plastic and liquid. The plastic limit is the water content where a soil

- in a semi-solid starts to exhibit plastic behavior.
- Reference measurements. Standard laboratory measurement methods used for soil characterization that are performed on sample subsets and then calibrated to soil infrared spectra for purposes of predicting values for the whole sample set. These are usually time-consuming and expensive analyses that are difficult or costly to perform on large numbers (thousands) of samples.
- Repeatability is the agreement between analytical results for the same sample analysed repetitively by the same operator using the same instrument. See also reproducibility.
- Reproducibility is the agreement between results from the same sample analysed repetitively using different instruments and operators. See also repeatability.
- SR. Sufficiency Range system for interpreting plant analysis results.
- SSN. Sample serial number. A sequential number assigned to samples logged into a laboratory. The number consists of a site code (e.g. S for Salien) followed by a number from 000,000 to 999,999.
- TXRF. Total X-ray fluorescence spectroscopy.
- USCS. Unified Soil Classification System classes soils for engineering purposed on the basis of particle size, gradation, plasticity index, and liquid limit (US Bureau of Reclamation 1960).
- USDA. United States Department of Agriculture.
- VNIR. Visible near infrared diffuse reflectance spectroscopy (wavelength range 350 to 2500 nm).
- XRPD. X-ray powder diffraction spectroscopy.

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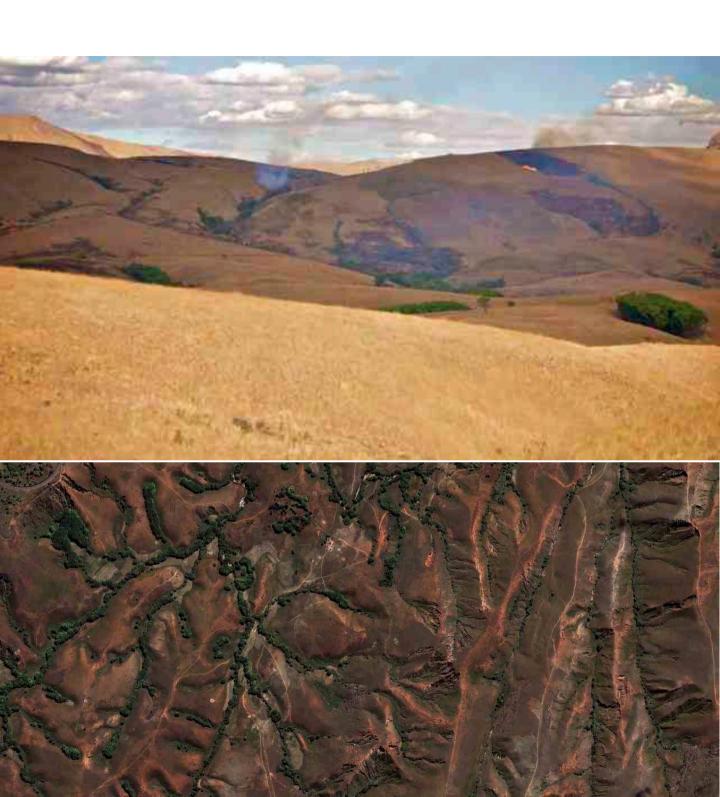
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4

Data Management

Geomatics is the multidisciplinary science and technology of gathering, storing, analyzing, interpreting, modeling, distributing and using georeferenced information.

It comprises a broad range of disciplines, including surveying and mapping, remote sensing, geographical information systems (GIS), and the global positioning system (GPS). These, in turn, draw from a wide variety of other fields and technologies, including computational geometry, computer graphics, digital image processing, multimedia and virtual reality, database management systems (DBMS), spatiotemporal statistics, artificial intelligence, communications, and Internet technologies among others.

In AfSIS, the above-mentioned disciplines form an integrated part of project activities. Large amounts of data are collected in field as part of the AfSIS field surveys, and large data sets containing soil reference data and infrared (IR) spectral signatures are generated in the laboratory. In addition, we collect and store data from existing soil legacy data archives (soil profile descriptions, etc). We also collect archived satellite imagery and new acquisitions of satellite data.

The sheer volume of data obviously requires appropriate computer hardware to manage, mine and analyze. However, computing power is not enough and clever approaches are needed for intelligently managing the data, as well as to find meaningful patterns and information (data mining).

In summary, the main types of data stored in AfSIS databases and archives include;

- Sentinel site survey baselines
- Infiltration data
- Soil data
 - Total X-ray fluorescence
 - X-ray diffraction
 - IR spectral data
 - Laser diffraction particle size data
 - Soil chemical data
- Satellite images
 - Quickbird / WorldView 2
 - Landsat (MSS, TM, ETM+)
 - ASTER
 - MODIS
 - NOAA AVHRR
- Other remote sensing (GIS) covariates
 - SRTM DEM and derivatives
 - ASTER GDEM
 - Climate data
- Soil legacy data

4.1 Data storage

The AfSIS databases have been developed on several platforms, but with the FileMaker database system as the central system for storage and data management (Figure 21).

We chose FileMaker because we needed a high performance database system that was able to handle tables with a large number of fields, and because one of our main requirements was a database system that is reasonably mobile and user friendly. The project has several nodes where NIR spectral data are stored and data-entry is conducted, and databases are hence distributed across regional laboratories. User friendly interfaces for data-entry have been developed using this platform.

Field data collection is conducted using GPS units running Windows Mobile installed, and the Cyber-Tracker software package (http://www.cybertracker.co.za). These data sets are ingested into the File-Maker database.

Open source databases

The AfSIS FileMaker databases are also mirrored in MySQL and PostgreSQL databases, and to some extent in SQLite.

MySQL (http://www.mysql.com) has become the world's most popular open source database. The main reasons for this are that it's easy to use, reliable and has consistent performance. It provides comprehensive support for application development, including stored procedures, triggers, functions, views, and cursors. MySQL also provides connectors and drivers (ODBC, JDBC, etc.) that allow all forms of applications to make use of MySQL as a preferred data management server. This is one of the principal reasons for the use of MySQL in AfSIS, and our efforts to build database-driven information systems.

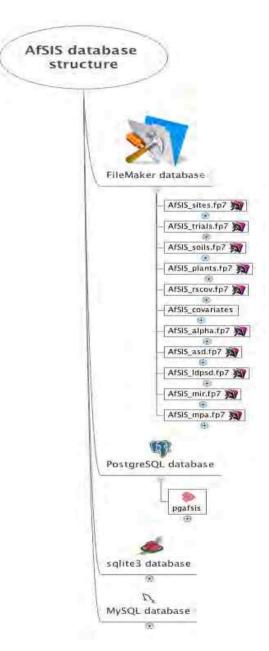


Figure 21. Schematic representation of the AfSIS database structure for field data, soil data, and spectral libraries.

PostgreSQL (http://www.postgresql.org) is a powerful, object-relational open source database system. It runs stored procedures in a number of programming languages, including Perl, Java, Python, Ruby, and Tcl, to mention some. PostgreSQL can also be extended with extensions and advanced features, including GiST (Generalized Search Tree) indexing, which is the foundation for PostGIS. PostGIS is a spatial extension that adds support for geographic information systems (GIS).

In addition we store some of our spatial databases in SQLite, which is completely self-contained, serverless, zero-configuration, and transactional. It reads and writes to ordinary disk files, and therefore en-

ables us to share databases, including spatial (GIS) databases across project locations in a simple way.

Satellite data

The AfSIS project has developed operational schemes for semi-automatic geo-matching and absolute radiometric calibration of Landsat and MODIS satellite image data, in collaboration with other scientists from the World Agroforestry Centre (ICRAF) in Nairobi, Kenya.

The raw and processed image archives are stored on a disk array, with off site tape backups. A hierarchical folder structure similar to that employed by

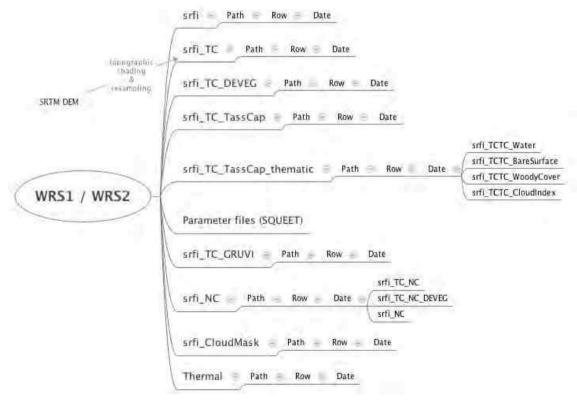


Figure 22. Overview of Landsat derived products held in the AfSIS image archives at the World Agroforestry Centre.

Landsat.org is used, as summarized in Figure 22.

The AfSIS remote sensing database holds data on indicators of land health derived from Landsat satellite imagery. These indicators can potentially be used for monitoring soil health across landscapes. The database also holds ground reflectance data for AfSIS sampling plots to be used in conjunction with spectral libraries and soil data for the development of prediction models and maps of soil health.

Some of the particular objectives include;

- implementation of automatic routines for converting Landsat raw image Digital Number (DN) data into metric indexes of absolute ground reflectance,
- development of intelligible indexes pertaining to biophysical ground conditions,
- identifying candidate compounded indicators for land health surveillance,
- creating a semi-automated processing chain that is accurate, internally consistent, relying solely on remote sensed imagery to produce indexes in a timely fashion.

AfSIS field database

The data collected in field during sentinel site surveys are stored in two tables - one containing the site baselines (158 fields) and another for the soil infiltration tests (13 fields). The structure of this database is shown in Figure 23.

An AfSIS unique plot ID field (primary key) is automatically generated using a combination of country code, letters (4) in the site name, cluster and plot (e.g. TZ.Chin.1.1). A function was written for the 4-letter site code to avoid duplication, starting by using the first four letters in the site name, then using combinations of other letters in the name if the first letters are taken.

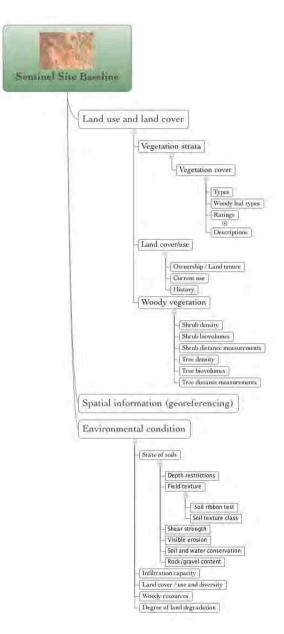


Figure 23. The AfSIS sentinel site field database structure, showing the the main variables stored.

AfSIS laboratory database

A relational database using FileMaker Pro (File-Maker, Inc.) is used for storing soil data. A data table holding details of the samples in the AfSIS soil database acts as a "node table" linking the various soil data tables (wet chemistry, carbon and nitrogen, cumulative mass, and IR spectral data) through a Sample Serial Number (SSN). The AfSIS plot ID is also stored in the sample details table and allows us to readily link these databases to the AfSIS field database, etc. (Figure 21). This relational database setup is illustrated in Figure 24.

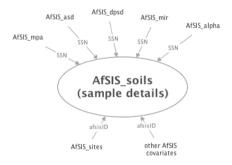


Figure 24. Illustration of the relational AfSIS soil database.

Soil reference data

The database schema for the soil reference database (AfSIS_soils) contains the following tables;

- table_SampleDetails
- table_SoilWetChem
- table_SoilCN
- table_TXRF
- table SoilCumMass

4.2 Building and maintaining spectral libraries

In AfSIS, a system for development and use of spectral libraries is used, as proposed by Shepherd and Walsh (2002) (Fig. 4) and later implemented as part of the Land Degradation Surveillance (LDSF) methodology used in AfSIS.

At the heart of this approach is the development of spectral library databases for NIR and MIR spectral data, respectively, as illustrated in Figure 24.

The approach involves a classic two-phase or double sampling strategy as follows;

- Sampling the Independent (Spectral) Phase:
 The variability of soils in a given study area is initially sampled thoroughly and characterized using IR spectroscopy. In the absence of additional information from soil maps, digital terrain models and/or remote sensing data, spatially stratified random sampling using spatial continuity functions is generally an efficient approach (Webster and Burgess, 1984).
- Sampling the Dependent Phase:
 Once the spectral variation of a target population has been thoroughly sampled, the more time consuming and/or expensive soil properties are measured on a subset of soils. Depending on the specific application, a variety of sub-sampling schemes may be used, ranging from equal probability to stratified- or design-based random sampling approaches.

Selection of calibration samples can also be done based on spectral diversity, as proposed by Shephed and Walsh (2002). Selection based on first derivative transformed spectra or baseline corrected spectra is often optimal to reduce the influence of albedo effects. There are several alternative ways of making the spectral selection. Most of them are based on use of principal component scores. Kennard and Stone (1969) proposed a sequential method that should cover the experimental region uniformly for use in experimental design. The procedure consists of selecting as the next sample (candidate object) the one that is most distant from already selected objects (calibration objects).

Terhoeven-Urselmans et al. (2009) used this approach while guarding against selection of samples from the same soil profile in calibration and validation sets. Other alternatives include use of clustering (Naes et al. 2002) or systematic sampling of

the principal component scores (e.g. Viscarra et al. 2008). Where an individual soil property is of interest and an existing calibration is available, predicted values of the property can also be used as a basis for selecting samples. Yet another approach uses weighting on bands known to provide information on properties of interest.

Shepherd and Walsh (2002) found that predictive performance of calibration models was improved when some randomly selected samples were included in the calibration, compared with systematic selection from the spectral data space alone. This improvement was hypothesized to be due to better sampling of the variation in the relationship

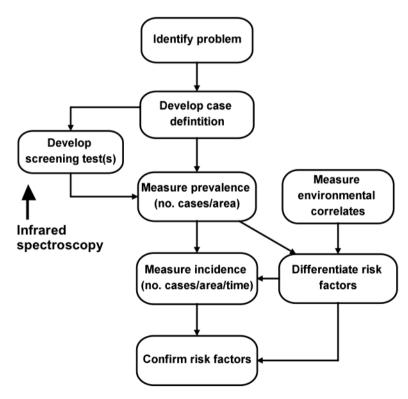


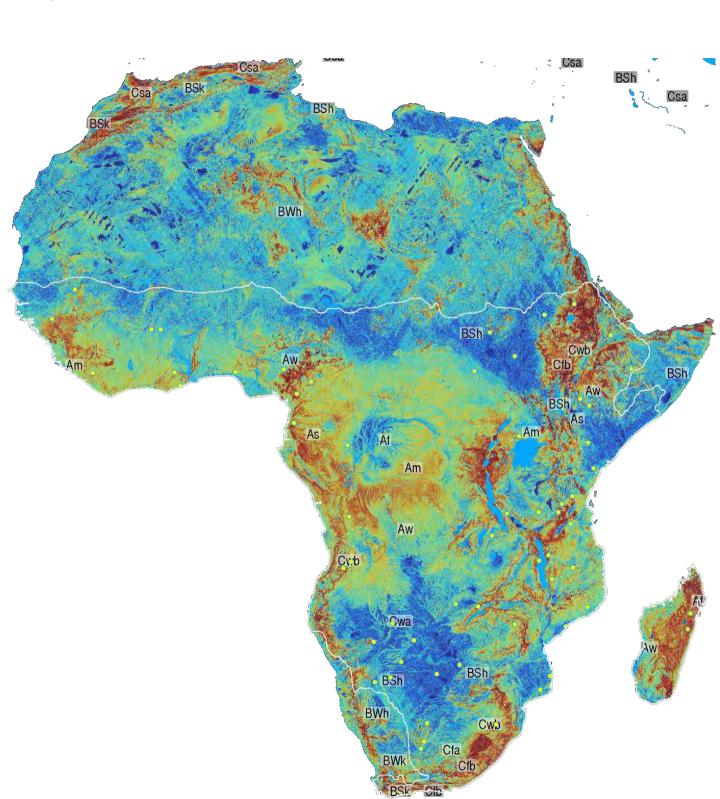
Figure 25. Logical scheme for use of reflectance spectral libraries in a risk-based approach to prediction of soil functional attributes. Source: Shepherd & Walsh (2002).

between soil properties and spectra. Hence sample selection based on a combination of geographic stratification and spectral diversity may be an optimal practice, as variation in soil forming factors such as climate, parent material and topography are sampled.

This approach can also be applied to the criterion for selecting new samples to add to a spectral library (Figure 25): selected samples from new geographic areas, not previously sampled (or from new strata based on geographic variables) are added to the calibration library even if the spectra are not detected as outliers with respect to the calibration library.

This procedure also permits inclusion of geographic variables as covariates or as to stratify the spectral calibrations, an approach that has considerable potential to improve prediction performance.





5

Data Processing and Interpretation

5.1 Data mining

Data mining is defined as the process of extracting patterns from data. Bayes' theorem and regression analysis represent early methods of identifying patterns in data (1700s and 1800s, respectively). It is therefore not a new technology, although the terminology is relatively recent.

In more recent decades there has been a prolific development of new methods for data mining as computer technology has evolved, including for example;

- neural networks
- clustering
- · genetic algorithm
- decision trees
- support vector machines

The four main classes of data mining tasks are; clustering, classification, regression and association rule learning.

Data

Data are facts, numbers, or text that can be processed by a computer. Including for example (in the context of soils) soil organic carbon concentration, cation exchange capacity or pH. Meta data, or data about the data itself are also data. Data generally refer to single instances or describe individual prop-

erties. Data are also generally quite easy to collect or obtain, although one could argue that this is not always the case - such as in AfSIS.

Information

Relationships, associations and patterns in data can provide information.

Knowledge

Knowledge is often difficult to find, and may be very time consuming to obtain as well. However, it is knowledge that allows us to make forecasts and predictions.

Intelligent data analysis

There are two categories of statistics - descriptive and inferential statistics. Descriptive statistics limit themselves to summarizing data, and in general no specific assumptions about the data are made. In inferential statistics on the other hand, more rigorous methods are employed that are based on certain assumptions about the data, and hence any conclusions drawn are only valid if these assumptions are

In the design of experiments we are generally conducting either an experimental or observational study. The main difference lying in whether we can control the data generating process or not, where in observational studies we have no control of this.

No matter what sort of study we are undertaking, intelligent data analysis may help us find answers to questions that arise by providing a set of steps or phases in the data analysis process. The initial phase in the process is **project understanding** - the main objective of the project being the primary thing to assess. In this phase, potential benefits, constraints, assumptions and risks should also be assessed critically. The next step in the process is data understanding, where the main objective is to gain general insights into the data that will hopefully be helpful in the next steps of the data analysis process. This will include understanding the *attributes* of the data being analyzed and assessing *data quality*. For these steps in the process it's important to "plot and look" and the data at hand using a range of visualization techniques.

Once we understand our data, including carefully checking whether they meet our assumptions, we can start looking at preparing the data for subsequent modeling.

5.2 Data modeling in AfSIS

The first step in the data modeling stage is to select the model class we want to use. In AfSIS we use several classes of models for the various types of data that we collect. The most important model classes applied are;

- Mixed-effects models
- Finite mixture models
- Multivariate calibration
- Classification

In the next sections we provide a rationale for the use of these model classes in AfSIS, and introduce them in more detail. Actual applications can be

found in training materials and publications emanating from the project.

Mixed-effects models

Grouped data are commonly found in many studies, and therefore occur in most areas of statistical application. Grouping structures can be simple or more complex, such as in nested or hierarchical designs, or may have a longitudinal or spatial structure. When data is grouped it is not appropriate to assume that observations are independent as the data will show correlations within the same group. The grouping structure can be modelled using *random effects*.

A mixed-effects model has both *random and fixed effects*. A simple example of such a model is a two-way analysis of variance (ANOVA). A model with a single level of grouping can be expressed as;

$$y_i = X_i \beta + Z_i b_i + \epsilon_i, i = 1, ..., M,$$
$$b_i \aleph(0, \Psi), \epsilon_i \aleph(0, \sigma^2 I),$$

where & is the fixed effects, b_i is the vector of random effects, X_i and Z_i are known fixed-effects and random-effects regressor matrices, and ε_i is the error term.

When we have multiple grouping levels, such as in AfSIS, it may have the following form;

$$y_{ijk} = \mu + b_i + b_{i,j} + \epsilon_{ijk}, i = 1, ..., M,$$

 $b_i \aleph(0, \sigma_1^2), b|i, j \aleph(0, \sigma_2^2), \epsilon \aleph(0, \sigma^2).$

where the site random effects b_i are assumed to be independent for different i, and the cluster within site random effects $b_{i,j}$ are assumed to be independent of the b_i . The within group errors $\epsilon_{\iota \phi \kappa}$ are assumed to be independent for different i,j, and k and to be independent of the random effects. See for example Pinheiro and Bates (2000) for a more thorough treatment of mixed-effects models, also including examples.

Hierarchical models are increasingly applied for analyzing natural resource data, and are particularly useful as soon as there is information about covariates at different levels of organization or scale.

For example, in studying the effects of soil management we may have information about individual soil profiles (e.g., changes in carbon content with depth), field-level information (management history, vegetation cover), and also information about land-scape setting (climate, parent material, topography). Another situation in which multilevel modeling arises naturally is in the analysis of data obtained by stratified or cluster sampling.

For example, in AfSIS 0.1 ha plots are nested within 100 ha clusters and 10,000 ha sites. Additionally, there may be repeated observations nested within sampling units, a situation that would arise when plots are monitored over time. With clustered (or longitudinal) sampling, multilevel modeling is in fact necessary in order to generalize model results to unsampled clusters in a population of sites.

The main reason that this is important in practice, is that model-based predictions that ignore differences in the spatial and/or temporal configuration of samples may be misleading. Estimates of the variability between sites and/or points in time, which are typically of central interest in management applications, would almost certainly be wrong.

There are additional features that make multilevel models useful in natural resource management applications. For one, sampling units do not have to be measured over the same number of points in time (and/or space), and thus units with incomplete data can be included in the analysis. This is an important advantage over classical methods that generally require complete data coverage.

Whereas classical approaches estimate only the average (or fixed) effects in a population, mixed-effects models can also be used to predict each sampling

unit. This are particularly useful in survey and surveillance studies where a proportion of subjects may deviate from the average (spatial and/or temporal) trend.

Finally, when combined with spatially contiguous data such as satellite images, digital terrain models and/or GIS data layers, mixed models can also be used for mapping.

Multivariate calibration

An important aspect of the LDSF and hence AfSIS is the extensive use of infrared (IR) spectroscopy in characterization of soil physicochemical properties, and the derivation of various indicators of soil condition or quality from IR spectral data (Vagen et al., 2006).

The use of traditional soil physicochemical analysis methods are costly and therefore limit effective sampling densities across landscapes. The use of IR spectroscopy allows us to characterize entire landscapes since it is both a cost-effective and rapid methodology, where the electromagnetic energy of molecular vibration is measured in a soil (or plant) sample.

Calibration

Sampling of the dependent phase is followed by a calibration step which describes the relationship between the reference property (y) and the multivariate spectral signal (xk), for example in linear form;

$$y = b_0 + \sum_{k=1}^{K} b_k x_k + f$$

where b0 and b are regression coefficients, k is the number of x-variables, and f is the y-residual.

The most commonly used calibration methods include multiple linear regression (MLR), princi-

pal components regression (PCR) and partial least squares regression (PLS) (Martens and Martens, 2001; Naes et al., 2002).

PLS and PCR are similar in that both employ orthogonal linear combinations of wavelengths to overcome the problem of high-dimensional, correlated predictors (multicollinearity) (Martens and Naes, 1989). PLS, the most widely used calibration method in infrared spectroscopy, orientates the components to the y variable.

Guidelines on treatment of calibration outliers are given by Naes et al. (2002). Only influential outliers are normally of concern, i.e. those with large leverage (distance in x-space) and large y-residuals.

Both PCR and PLS are now available in most standard statistical packages (e.g. Genstat, S-Plus, SAS, R) as well as in more specialized "chemometric" software packages, such as The Unscrambler® (Camo Inc), Matlab (The MathworksTM), PLS-Toolbox (Eigenvector Research Inc), and ParLes (Viscarra Rossel, 2008). Additionally, non-linear regression methods (e.g. generalized additive models and regression splines, local PLS), and non-parametric classification and regression methods (e.g. classification and regression trees, neural networks, support vector machines, genetic algorithms) have also been successfully used in past soil reflectance studies.

Scripts, functions and libraries for R-statistics (http://www.r-project.org/) are under continuous development and several spectral processing and regression tools are available in the R package "soil. spec" (http://cran.at.r-project.org/).

Validation

Regardless of the specific technique employed, the most important aspect in developing robust predictive models is to ensure that model validation

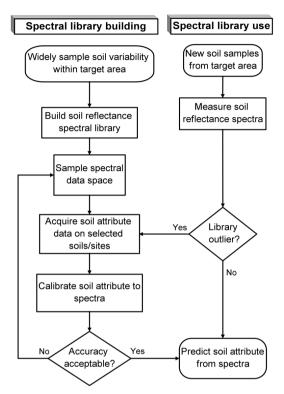


Figure 26. Logical scheme for use of reflectance spectral libraries in a risk-based approach to prediction of soil functional attributes. Source: Shepherd & Walsh (2002).

matches the intended model use. Model validation in this context simply means checking how well the model will perform in predicting new data. The simplest measure of the uncertainty on future predictions is the root mean square error of prediction (RMSEP). This value expresses the average uncertainty that can be expected when predicting the response-values for new samples (see Naes et al., 2002). RMSEP is valid, provided that the new samples represent an independent sample of the population under consideration; otherwise, the actual prediction errors might be much higher. In this case, the term "independent" refers to the notion that knowing something about the validation samples would not be helpful in predicting

the response-values of the calibration samples. Soil samples taken in close proximity to one another or at different depths in the same soil profile are typically not independent of one another and their inclusion in both calibration and validation sets can lead to over-optimistic validation performance.

Other metrics for evaluating prediction performance commonly used include the ratio of prediction to standard deviation (RPD) and the ratio error range (RER). These are calculated as (a) the standard deviation of the reference measurements in the validation set, or (b) the range of the reference measurements in the validation set, divided by the standard error of prediction, respectively. Guidelines on interpretation are given my Malley et al. (2004). Standards for multivariate calibration are given in Standard Practices for Infrared Multivariate Quantitative Analysis (ASTM E1655-05) and Standard Practice for Validation of Empiricially Derived Multivariate Calibrations (ASTM E2617-08a).

Cross-validation is commonly used to evaluate calibration model performance and prevent over-fitting, however, cross-validation does not substitute for use of independent validation sets in evaluating model performance. Statistical re-sampling or ensemble techniques such as bootstrap aggregation (or bagging) have also been employed to improve prevent over-fitting, stabilize models and improve prediction accuracy (e.g. Vicarra Rossel, 1997; Brown et al., 2006).

Soil classification problems, where the y-variable is discrete rather than continuous can be calibrated using modifications of many of the same calibration methods, for example using discriminant PLS or classification trees. Examples of soil diagnostic screening tests are given by Shepherd and Walsh (2002). Unsupervised classification of spectra have also been used to produce spectral classes, which are then interpreted in terms of soil properties (e.g. Vagen et al., 2006).

Figure 27. Example showing prediction of soil organic carbon (SOC) from NIR spectral data using a multilevel PCR model.

Data pre-treatment

Various signal processing or spectral data pretreatment, such as smoothing and filtering, transformation, standardization, and numerical treatment are used to improve signal-to-noise-ratio, correct for light scattering, convert data into more physically meaningful form, and extract meaningful or useful information before calibration.

First derivative processing and smoothing have been found to be generally optimal for calibration of many soil properties. Wavelet transforms have shown promise as a way to simultaneously optimize soil spectral information, reduce data volume and solve multicollinearity problems (e.g. Ge et al., 2007; Viscarra and Lark, 2009). Continuum removal (Clark and Roush, 1984) is useful for maximizing information on absorption features and may be worth further study.

Transformation of the y-variable is usually also necessary to obtain normally distributed data in order to satisfy the assumptions of parametric methods and to help minimize non-linearity in calibrations. Soil element concentrations are typically highly skewed due to a low frequency of large values. Performance statistics are calculated on the back-transformed values. Prediction errors can be calculated for windows across the range of the reference values, and the probability of predicted values being above or below critical limits can also be calculated.

Classification

Classification problems arise in cases where the aim is to assign each input vector to one of a finite number of discrete categories. In cases where we are interested in modeling dependency towards one particular attribute, or where we have access to a value for the target attribute, the latter is often referred to as *supervised learning*.

We apply various classification methods in AfSIS;

Decision Trees - involve a hierarchical way to partition the input space to explain how different areas of the input space correspond to different outcomes.

Bayes classifiers - use simple probabilities to express their model.

Regression models - form the counterpart to numerical approximation problems. Unlike other approaches where the aim is to find a classifier and minimize the classification error, the approach in regression models is to minimize the approximation error.

Rule models - these are generally not the first choice for classification since not many usable algorithms exist for complex data.

Figure 28. Example of the use of finite mixture models for the development of soil condition classes in Segou region, Mali (Vagen et al, in print).

Finite mixture models

Finite mixture models are applied in a wide range of areas for modeling unobserved heterogeneity or for approximating general distribution functions (McLachlan and Peel, 2000).

In AfSIS we use finite mixture models in model-based clustering (see example in Figure 28). The use of such probability models, rather than heuristic procedures, for clustering is becoming more and more common for image segmentation and in a number of other applications, including the analysis of IR spectral data.

We use model based clustering methods in analysis of IR spectra to estimate a model for the data that allows for overlapping clusters, as well as a proba-

Index	Туре	Algorithm	Biophical interpretation
Simple ratio (SR)	Band ratio	VIS/NIR or SWIR/NIR	Vegetation index
NDVI	Band normalization	(NIR-VIS)/(NIR+VIS)	Vegetation index
SAVI	Band normalization with corrections	(NIR-VIS)*(1+L)/(NIR_VIS+L)	Vegetation index
EVI	Band normalization with corrections	(NIR-VIS)/ (NIR+C1*VIS+C2*BLUE+L)	Vegetation index
NDSI	Band normalization	(VIS-SWIR)/(VIS+SWIR)	Snow and ice indexing
NDWI	Band normalization	(NIR-SWIR)/(NIR+SWIR)	Water and burnt area indexing

Table 3. Pixel-based indices derived from ratios and normalizations of 2 image bands.

bilistic clustering that quantifies the uncertainty of observations belonging to components of the spectral mixture.

5.3 Remote sensing

In recent years time series of moderate resolution satellite imagery such as Landsat have become available free of charge. This has allowed for operational monitoring of forest changes using Landsat data.

Many indicators of environmental health (ecosystem status) can be derived from remote sensing, either alone or in combination with ancillary data. For large, data poor regions, remote sensing presents the best option for monitoring and surveying ecosystem status.

An index is any remote sensing derived parameter that is unambiguously defined, preferably on a metric basis. An index can also be an indicator, if it is corroborated as carrying relevant and desired information. An indicator, however is more likely to be defined as a compound of two or more indices, or from a combination of indices and ancillary data. Indicators should be intelligible, and preferably defined in metric units, but they can be non-metric.

In general, indicators simplify complex phenomena. However, they do not reduce complexity. Environmental indicators are developed around the concepts of drivers, pressures, state, impact, and responses (the DPSIR model).

In satellite remote sensing single band reflectance is a metric index, but carries limited meaning (at least for the non-expert). A normalized vegetation index is dimensionless, but nevertheless a better indicator of vegetation density compared to single bands.

To qualify as an indicator the following criteria should be considered (Rice 2003):

- Meaning
- Ability to measure
- Accuracy/precision
- Representativeness
- Availability of historic records
- Specificity
- Ability to be used as reference
- Sensitivity
- Responsiveness
- Theoretical basis

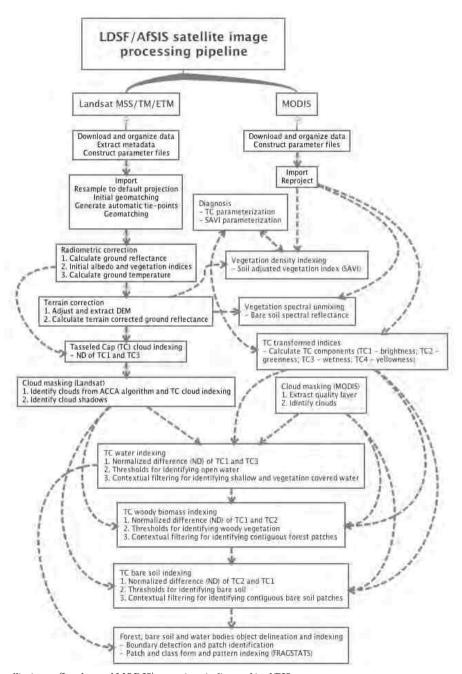


Figure 29. Satellite image (Landsat and MODIS) processing pipeline used in AfSIS.



Figure 30. Watershed map of Africa derived from the filled SRTM DEM.

Traditionally, remote sensing analysis often centers on deriving various indices (e.g. NDVI), spectral unmixing techniques, and classification. The approach taken in AfSIS, which builds on studies conducted using the LDSF methodology during the last 5 years, is somewhat different from conventional remote sensing analysis in that we take more of a statistical approach.

We take various indices developed along with raw data (e.g. ground reflectance) and combine these with our sentinel site ground data in order to develop models that allow us to predict for example tree density across landscapes, and various soil related properties.

For this type of approach to be successful, however, the processing of the imagery used to develop the covariate database is critical. A lot of emphasis has therefore been on pre-processing and processing of the image sensor data to create data sets that allow us to derive models at continental scales where we are combining data from thousands of Landsat scenes for example.

Vegetation cover

Vegetation cover is essential for the functioning of local ecosystems, for land health and for the water cycle, and at the global scale it also affects the carbon cycle and climate. To date, regional to global vegetation change detection has relied on coarse scale imagery, with early attempts focusing on the National Oceanic and Atmospheric Administration (NOAA) operated Advanced Very High Resolution Radiometer (AVHRR) series of sensors (Malin-



Figure 31. Perpendicular Vegetation Index (PVI) image from the Rift Valley in Kenya. Lake Nakuru is in the center of the image. Dark brown is bare; Dark green is dense vegetation.

greau and C.J. Tucker, 1988; Myneni et al., 1997).

More recently, Moderate Resolution Imaging Spectroradiometer (MODIS) data (Hayes et al. 2008) have been increasingly employed. The finest-scale global data set is the global Continuous Vegetation Fields (VCF) datasets from MODIS at 500 m spatial resolution (Hansen et al. 2003).

Reliable data at higher resolution are urgently needed both for a better scientific understanding of the relations between vegetation cover and soil, water and climatic conditions at different scales, for relating local socioeconomic conditions and land health, and for sustainable land management.

Potential users of such data also include the UN Convention to Combat Desertification (UNCCD), the Convention on Biological Diversity (CBD) and the Ramsar Wetland Convention, as well as the Intergovernmental Panel on Climate Change (IPCC).

Creating an operational framework by adopting Landsat data for automated mapping is urgent in Africa, where land cover change and deforestation is caused largely by shifting agriculture, and is therefore highly fragmented.

The need for more high-resolution data is also evident in the well known discrepancy between estimates of deforestation derived from ground data, and those derived from past coarse-scale satellite image surveys. Also, the changes captured by coarse resolution imagery is generally not relevant to the scale at which land management is taking place, hence one will not be able to pick up properties sensitive to management.

Hierarchical analysis

In AfSIS we use a spatiotemporal hierarchical scale for land health monitoring, ranging from coarse to fine resolution as follows;

- 1. continental to river basin,
- 2. hillslope (watershed),
- 3. patch (or stand), and
- 4. ecotope (single tree)

The continental scale is simply delineated from global datasets of coast lines, from a hydrologically adjusted (filled) version of the Shuttle Radar Topography Mission (SRTM) data (available for download here; http://africasoils.net/data/rsdownload), and the major river basins of Africa delineated from the filled SRTM DEM above (Figure 30).

The watershed map can be used for segmentation of AVHRR and MODIS derived indices and indicators to river basins. Refinements are needed for some regions.

Patches are defined as uniform ecological stands, and can be delineated from e.g. vegetation maps. The processing chain presented in Figure 29 automatically generates patches of forests, non photosynthetic vegetation, bare soil and water from Landsat (28.5 to 57 m resolution) and MODIS (500 m resolution) multispectral data.

Data processing

Processing of multi-date satellite imagery is highly demanding and comprises several steps, including;

- 1. calibration to radiance or reflectance
- 2. atmospheric correction
- 3. image geo-matching
- 4. terrain correction
- masking of clouds and cloud shadows and other unwanted features.

A data preprocessing chain for geometric and radiometric calibration of Landsat data, and a processing chain for index generation that can use both MO-DIS and Landsat data as input has been developed and is being applied in AfSIS (Figure 29).

Once corrected and calibrated, the data can be used for calculating relevant indices that can be compared over time.

Pre-processing

Data from MODIS, AVHRR and other wide swath image sensors need special attention for radiometric correction due to view angle variations and varying atmospheric depth. The MODIS and AVHRR products are already corrected using a bidirectional reflectance distribution function (BRDF), and are hence free from view angle effects and with cloud and aerosol contamination encoded. Landsat data and other higher resolution data have negligible errors stemming from view angle effects.

In AfSIS, we apply a semi-automated procedure for georeferencing Landsat data using a ground control point-matching script. For each WRS position the Global Land Survey (GLS) 2000 Landsat ETM data set is used as a template for both projection, resolution and georeference.

The MODIS data is resampled and reprojected using the MODIS Reprojection Tool (MRT), with the native georeferencing accuracy accepted.

Relative radiometric calibration can be done from a (full) scene based on simple regression (SR) normalization, or based on pseudo-invariant-features (PIF).

Absolute radiometric calibration either uses ancillary data or derives the atmospheric corrections from the scene properties itself.

Relative calibrations are in general easier to apply, and reported to perform equally well as the absolute algorithm. Identifying pseudo invariant features is the major obstacle in PIF normalization. Truly invariant targets can only be identified in hyper-arid regions, although dense forests are also frequently used as pseudo-invariant-features.

In order to make satellite derived reflectance metrics directly comparable with field and laboratory derived reflectance data, absolute calibration methods are called for.

Processing of calibrated and georeferenced Landsat and MODIS reflectance data

After georeferencing and radiometric calibration the Landsat and MODIS reflectance data enter the processing chain (Figure 29) using the same algorithms, only differing in the parameterization on the tasseled cap components.

Pixel-based indices

These are simple indices often based on band ratios and normalizations (Table 3). In AfSIS we derive several pixel-based indices as part of automated image processing pipelines and later explore these as covariates in relation to ground data from the sentinel site surveys (see section 5.1).

An alternative set of indices is also derived to explore the spectral domain more fully. With these indices and optimal soil line is identified prior to normalization, and they can therefore be calibrated to have better physical correlation with vegetation density. Both these indices are calculated as part of the image calibration pipeline applied in AfSIS, and stored with the surface reflectance (SRFI) rasters.

These so-called n-space indices include;

- the Perpendicular Vegetation Index (PVI)
- the Perpendicular Brightness Index (PBI)

Object oriented analysis

The patch is defined as a piece of the landscape that is considered homogeneous at the scale of a particular study, and is the basic unit in landscape ecology. A landscape is comprised of a mosaic of different types of patches.

In AfSIS we apply the FRAGSTATS program (Figure 29) to calculate a number of statistics for patches in landscapes, and for the landscape as a whole. FRAGSTATS is concerned with both landscape composition and landscape configuration. Landscape composition addresses the variety and abundance of patches within the landscape, while landscape configuration is concerned with physical distribution and spatial character of patches.

Challenges and constraints

The low repeat cycle of moderate to high resolution imagery, combined with persistent cloud cover, sensor drift, atmospheric disturbances, sensor malfunction (e.g. SLC off of the Landsat ETM+ sensor as of May 2003) present some challenges and limitations for their application in change detection studies. Another constraint is data quality, particularly when there are sensor malfunctions.

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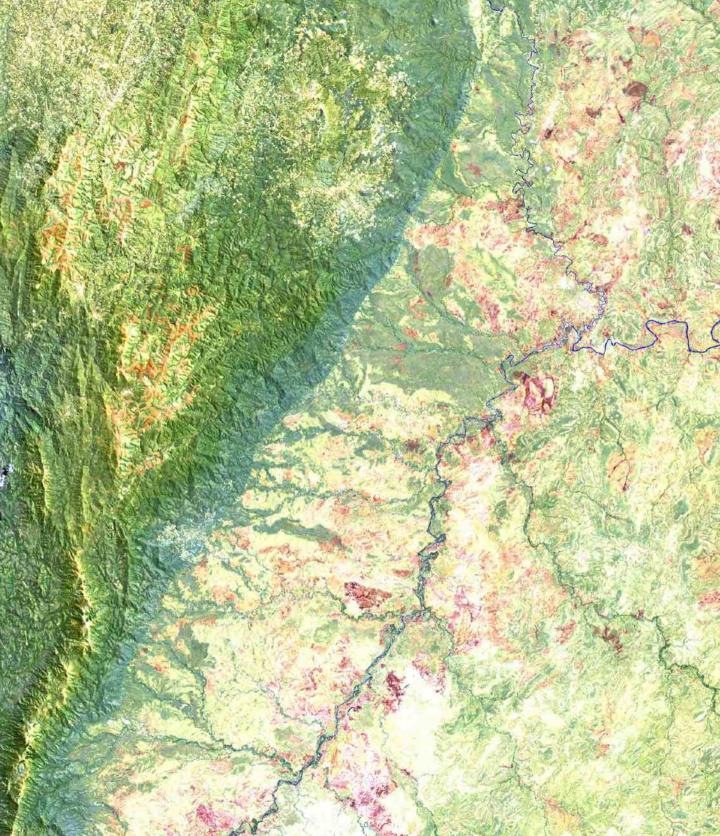
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