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Diffusive reflectance spectroscopy for precise analysis of soils: An overview

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Abstract
Soil testing plays a vital role in modern agriculture, helping in optimizing crop yield and sustainable land management. Traditional methods are often labor-intensive and time-consuming, which lead to the exploration of rapid alternatives such as diffusive reflectance spectroscopy [DRS]. DRS focus on the interaction of light with materials, utilizes the diffusely reflected radiation to glean insights into the optical properties of the sample. Unlike specular reflection, diffuse reflection occurs in all directions, making it ideal for analyzing rough-surfaced materials like soils. DRS instruments are equipped with integration spheres or diffuse reflectance attachments, they measure the spectral reflectance properties of soil samples, with optical fibers facilitating transmission to the spectrometer for analysis. In soil testing, DRS offers rapid and non-destructive assessment of soil properties. It estimates nutrient levels, organic carbon content, clay minerals, soil moisture, and salinity by exploiting the unique spectral fingerprints of soil constituents. This facilitates informed decision-making regarding fertilization, irrigation, and soil conservation practices. Future research aims to enhance the precision and feasibility of DRS in agriculture. Combining visible near-infrared [VNIR] and mid-infrared [MIR] spectra improves predictive capabilities, while calibration using spectral data from smallholder farms enhances model accuracy. Standardization of methods and protocols is crucial for ensuring consistency and reliability in soil testing procedures. Despite its benefits, DRS presents challenges in soil analysis. The complex and variable nature of soil matrices complicates the development of accurate calibration models, requiring standardized procedures and reference materials. Additionally, the need for a large number of samples and expertise in data processing may hinder widespread adoption of DRS in soil science.

Keywords: Soil testing, diffusive reflectance spectroscopy [DRS], non-destructive analysis rapid analysis, optical properties

Introduction

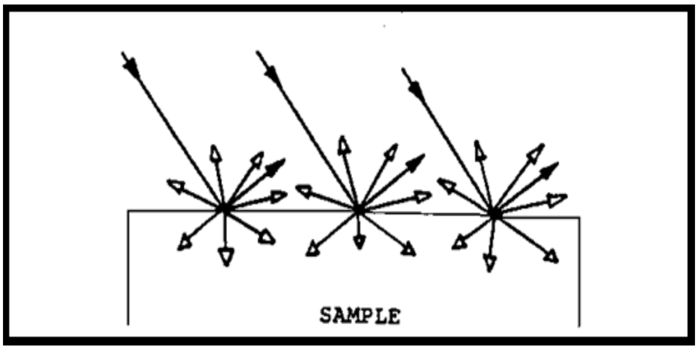
Techniques of soil testing in order to increase the crop yields and production scales become very necessary now a days to ensure the soil health balance and food security. Soil testing techniques focuses on the common goal of identifying the nutritional stress in soil and helps farmers to make well-informed fertilization decisions in order to establish a nutrient management plan for specific crops [1]. Conventional approaches of soil testing frequently include chemically extracted nutrients from the soil and comparing the amount extracted to the reaction of plants [2]. The amount of nutrients measured by various soil tests can vary substantially depending on the kind of extractant used, and thus interpreting a soil-test value requires understanding of the effects of the extractant used, soil sampling technique, sample handling and the intended application of the result [3]. However, these methods often require sample preparation steps and can be time-consuming. Recently, there has been rapid soil testing methodologies, which provide faster and more efficient ways to measure the soil nutrients content. Rapid soil nutrient assessment relies on spectroscopy-based methods such as X-ray fluorescence [XRF], mid-infrared [MIR] and near-infrared [NIR] [1]. One such technique is Diffusive reflectance spectroscopy [DRS] in NIRS [near-infrared reflectance spectroscopy]. This is especially useful in scenarios which requires a large number of studies and samples or when the primary [conventional] analytical approach is time-consuming and costly such as for high-resolution digital soil mapping or precision agriculture [4, 5]. Using DRS, one can easily gathers and analyze the dispersed infrared energy to quantify the extremely minute particles or coarse surfaces.

In spectroscopy, scattering is frequently dependent on well-designed optical contrast agents such as gold nanoshells [6]. The diffuse reflection of photons in the ultraviolet to visible range [190-800 nm] of a material is measured using a spectroscopic technique known as DRS. When there is negligible dispersion and the angle of incidence and reflection is exactly equal*i.e.* specular reflection, this method is used to analyze solid [thin film] and liquid materials [7]. For instance, a single reflectance spectrum can be used to assess the wide range of soil variables, including fundamental soil qualities parameters, soil classification, nutrient contents, mineralogical composition, weathering indices, solute transport parameters, organic matter content, mineralogy and other properties can be obtained [8,9,10,11,12,13].The DRS approach is appealing due to its rapidity, environmental friendliness, non-invasiveness and its ability to collect the DRS data from both onboard remote sensing systems and proximal sensors [14]. As molecules and atoms absorb light at certain wavelengths and have distinct spectra, diffuse reflectance spectroscopy is a long-standing quantitative approach in physical and analytical chemistry [15]. Therefore, the present reviewsexplain the concept of diffusive reflectance spectroscopy in soil testing with the view of future aspects in agricultural sector.

Principle of diffusive reflectance spectroscopy:

When light strikes a material, it interacts with both its surface and its underlying layers. Hence, the substance absorbs light, transmits it and reflects some of it back. The amount of light reflected is determined by the optical properties of material, which include absorption, scattering and its reflection coefficients [16].The diffuse reflection phenomenon iscritical for collecting the representative data on the optical characteristics of materials. Many factors influence these properties including the material's composition, structure and surface form. Understanding these optical qualities is critical for many applications [17, 18]. Founding principles of DRS provides a robust platform for investigating these characteristics in an adaptable and non-destructive manner. As the dispersion inside the material, light in diffusive reflectance spectroscopy is diffusely reflected in all directions rather than specularly reflected [reflected at the same angle as the incident light]. The microscopic rough surface of material scatters light in numerous directions, which accounts for its diffuse reflection. In figure 1, the shaded arrows represent the spectrum reflection which is radiation with an angle of reflection equal to the angle of incidence. Diffuse reflection is defined as radiation with an angle of reflection that is independent of the angle of incidence, and it is shown by empty arrows [19].

DRS is used in materials research to characterize a variety of materials, such as semiconductors [20], polymers and nanoparticles [6].



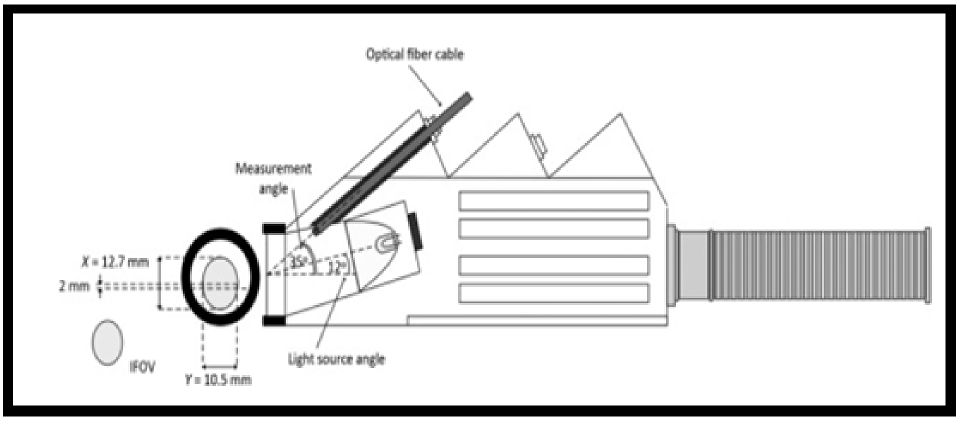
Source: Diffusive Reflectance spectroscopy by Jonathan P. Blitz

Fig 1: Spectrum reflection and diffusive reflection by the sample

Soils differ from vegetation in that they are complex mixtures of organic and mineral elements, with distinct spectral fingerprints. The shape of soil spectral fingerprints is influenced primarily by iron and organic matter concentrations as well as moisture and salt content [21, 22].When the reference measurement contains a significant inaccuracy, DRS can provide results with greater precision and accuracy than the actual measurement. As a result, it is expected that DRS will have higher laboratory reproducibility than standard analysis methods. DRS has several advantages, including its speed of analysis and ability to estimate several soil properties from a single robust test, which is especially useful for soil variables that require a long time to measure using standard methods [23]. This might be extremely advantageous in terms of minimizing the time and effort required to transfer the samples, particularly in areas where laboratory facilities are not easily accessible. Furthermore, it would considerably reduce the need to send samples that may be contaminated with illnesses and insects [24].

Diffusive reflectance spectroscopy instrumentation and measurement techniques

For soil testing through DRS, the equipments and instrumentation are specifically designed to measure the spectral reflectance properties of soil samples across various wavelengths. There are several instruments in this method. For instance, spectral radiometers or spectrophotometers are the primary instruments used to measure the reflectance spectrum of the soil samples. The spectral measurement can took place in field as well as in the laboratory. The difference between both is the source of light, where in field, the source of light is the sun, whereas in the laboratory, it have artificial source of illumination. Laboratory spectrophotometer is typically a tungsten halogen lamp or a deuterium-halogen lamp capable of emitting light across a broad spectrum of wavelengths often spanning from ultraviolet [UV] to near-infrared [NIR] regions. It measure the intensity of light reflected from the soil sample over the specified wavelength range [25]. In Fig. 2, In the study by Lamine S., *et al.* [23], the probe body is positioned at a 12° angle with a 100 W reflectorized halogen lamp and the detected spot has a diameter of 1.1 cm and a field of view of 1.33 cm^2. In this case, the spectrum was gathered using a high-intensity contact probe [CP; direct contact with the soil]. A black plastic dish the size of a Petri dish was filled with earth particles less than 2 mm. The CP was then brought into direct contact with the dirt, and the spectra were recorded.



Source: Hyperspectral remote sensing by Salim Lamine *et al*.

Fig 2: Laboratory spectral radiometer

To ensure the accurate measurement of diffuse reflectance, DRS instruments for soil testing often incorporates an integration sphere or a diffuse reflectance attachment. This component diffusely reflects the light onto the soil sample, ensuring the uniform illumination and minimizing the effects of sample orientation and surface roughness on the measured reflectance [26]. Also, optical fibers or fiber optic probes are used to guide the reflected light from the soil sample to the spectrometer or radiometer for analysis. These fibers are typically designed to transmit the light efficiently across the desired spectral range while minimizing signal loss or distortion [Kane, 2024, 27]. Furthermore, calibration standards and reference materials are essential for ensuring the accuracy and reliability of DRS measurements. These standards may include materials with known reflectance properties, such as Spectralon® or $BaSO_4$ [barium sulfate] panels or white russian opal glass which are used to calibrate the instrument and validate measurement accuracy [28].

Applications of NIRS in soil testing

This method estimates and characterizes these attributes by using the reflectance characteristics of soil samples. The following is how some soil parameters are predicted using NIRS

a) **Soil salinity:** Through the use of visible-near infrared reflection spectroscopy bands to detect the surface soil salinity, NIRS has been utilized to assess the changes in soil salinity at various scales [29]. Hyperspectral data, including NIRS have been employed for the quantitative assessment of soil salinity and other soil properties [30, 31]. NIRS can reliably predict the soil salinity by exploiting the relationship between the soil characteristics such as moisture and salt [32].

b) **Organic Carbon:** NIRS has been used to predict the soil organic carbon [SOC] content. Assessing the greenhouse gases [GHG's] emission from soils requires precise knowledge of the nitrogen and carbon cycles [33]. Near-infrared reflectance spectroscopy [NIRS] is a quick and non-destructive method for estimating the quantity of organic carbon in soil in the near-infrared range [1000-2500 nm]. It has been discovered that decision-tree modeling paired with visible-NIR spectroscopy may accurately estimate soil organic carbon with little to no uncertainty [34].

c) **Clay Minerals:** Understanding the qualities and presence of clay minerals in soil is critical for knowing their properties and behaviors. Clay minerals play an important role in soil structure, water retention and nutrient absorption. Spectroscopic techniques like NIRS can potentially be used to analyze and identify the clay minerals in soil samples based on their unique spectral signatures [35].

d) **Soil moisture:** The inverse relationship describes how the reflectance decreases as soil moisture content increases. This alliance can be the result of two factors: water on the lattice sites of some minerals in the soil and thin coatings of water covering soil particles [36]. The shift in spectral reflectance caused by variations in soil moisture levels became more visible at longer wavelengths [>1450 nm] as measurement tools developed [37].

Future directions and emerging trends

The primary goal of current research trends and breakthroughs in this subject is to improve the precision, effectiveness and feasibility of diffuse reflectance spectroscopy [DRS] for soil testing in agricultural applications. Combining visible near-infrared [VNIR] and mid-infrared [MIR] spectra has shown promise in boosting the effectiveness of DRS for soil testing and researchers are looking into how to improve the chemometric models using this method [38]. More emphasis is being put on calibrating the chemometric models using spectral data from smallholder farms to improve the forecast accuracy and testing DRS models with appropriately sampled datasets to ensure reliable results [39]. DRS is being compared to standard wet chemistry-based soil testing procedures to determine how well it performs in terms of cost-effectiveness, dependabilityand nutrient recommendations [39, 40].

Using DRS data to construct the soil quality indexes [SQI's] is gaining popularity as a comprehensive approach of evaluating soil quality that takes into account a range of soil characteristics to help with soil management decisions [41]. DRS technology is increasingly being employed on smallholder farms, with a focus on fast soil testing and fertilizer recommendations to combat the soil degradation and to increase farm revenue [41].

Challenges and limitations

Besides the several uses of DRS in NIRS, there are still some numerous problems associated with it. NIRS analysis is more difficult than plant analysis because the soil matrix is so complex and variable.As soils are so variable, and therefore, developing trustworthy and repeatable calibration models for precise soil parameter predictions may be difficult [42]. When employing NIRS for soil analysis, differences in sample preparation and reference procedures between studies can lead to conflicting results. To improve the consistency and reliability of NIRS forecasts, reference methodology and sample preparation procedures must be standardized [43].

Also, to make accurate predictions and account for sample variability, a large number of samples are required to create robust calibration models for NIRS analysis of soils [44]. Calibrations based on a short sample size and insufficient validation may result in less accurate predictions. Apart from these, some other challenges are there such as lack of equipments in laboratory, insufficient knowledge to effectively conduct measurements, complex data processing and absence of standardized procedures and protocols for soil spectroscopy analysis can hinder consistency and comparability of results [45].

Conclusion

In conclusion, diffusive reflectance spectroscopy [DRS] provides a rapid, non-invasive and effective analysis of soil properties, making it a promising advancement in soil testing procedures. DRS uses the rules of light interaction with materials to characterize the soil samples at various wavelengths, providing valuable information on mineralogy, organic matter content, nutrient levels and other important soil parameters. Spectral radiometers, integration spheres, fiber optic probes and calibration standards are just a few of the tools and measurement methods utilized in DRS to ensure the precise and consistent data collection in both lab and field settings. Furthermore, DRS's versatility allows it to estimate the soil parameters such as salinity, moisture content, organic carbon and clay minerals facilitating well-informed agricultural practice decisions. DRS have numerous advantages, but it also has certain limitations and challenges. As soil matrices are complex and varied, it is difficult to develop trustworthy calibration models and thus standard operating procedures and protocols are essential to provide consistent results. Furthermore, the need for a large number of samples, as well as understanding of data processing and interpretation, may limit the broad application of DRS in soil analysis. In the long run, initiatives to increase the accuracy and efficacy of DRS for soil testing are underway. These include initiatives to standardize the measurement techniques, aggregate spectral data from many places and calibrate models with varied datasets.

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