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Review

Vibrational spectroscopy in soil and sediment analysis

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ABSTRACT

The literature concerning the use of vibrational spectroscopy for soil and sediment analysis, published in the last years, has been revised in order to provide a picture of the strengths and weaknesses of these direct techniques to characterize soil composition and properties. Many soil components as water, organic matter, like humic substances, and minerals, can be determined together with physicochemical parameters as pH, conductivity or redox potential. The main strategies to obtain sample spectra and to extract, as many as possible, useful information were evaluated, taking into account the progress on chemometrics and discussing the whole analytical process, from sampling to sample preparation, spectrum measurement and data treatment.

Contents

1. Soil and sediment analysis

Soil is the main component of the solid biosphere, populated by various organisms from bacteria to plants, animals and humans and it provides the most characteristic features of the terrestrial environment. The main properties of the soil are its fertility or bioproductivity. This parameter depends on physical parameters; such as soil depth and texture, together with chemical composition (pH and content of various nutrients) and physicochemical properties; such as water absorption capacity [1].

Soil is a mixture of minerals, water, air, and living organisms that are usually classified according to the mineral particle size as: (i) clays, lower than 2 μm, (ii) silts, from 2 to 20 μm, (iii) sands, from 20 to 2000 μm, and (iv) gravel, bigger than 2 mm. Fig. 1 shows the classification of the US Department of Agriculture (USDA) of the different types of soils as a function of the mixtures of the aforementioned particles in different proportions [2].

The chemical composition of silt and sand is generally dominated by quartz. Calcite, $CaCO_3$, and dolomite, $CaMg(CO_3)_2$, may predominate in areas where the soil was formed from limestone. In the tropics, Al and Fe oxides and hydroxides dominate in these fractions as a result of more intense weathering. The clay fraction is composed mainly of clay minerals (kaolinite, montmorillonite, . . .), humic substances and oxides of Al and Fe [3].

On the other hand, sediments are formed in water bodies as a result of the settling of suspended matter. Considerable sedimentation takes place in estuaries, where there is a reduction in the river flow velocity due to mixing with seawater and this can result

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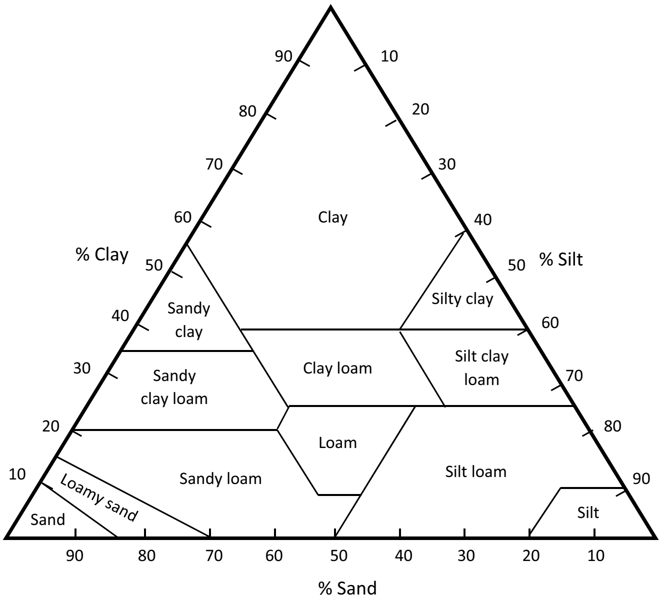

Fig. 1. Three phase diagram of soil composition as a function of the proportion of clay, sand and silt (Extracted from Ref. [1]).

in the formation of muddy tidal flats. Since these particles originate at the surface of the water body, sediment cores can reveal chemical changes that have occurred in the environment in the past [4], thus, providing a memory of the water and soil pollution.

Unfortunately, soil resources are being irreversibly lost and degraded at an unprecedented rate as a result of increasing and often conflicting demands coming from nearly all economic sectors, including agriculture, industry, construction, tourism and transport and these human activities have dramatically affected the quality and composition of soils and sediments. Maintaining good soil quality and minimizing soil and sediment pollution and degradation is of fundamental importance to (i) protect our food supplies from toxic substances, which can be accumulated in the soil and enter the food chain, (ii) preserve groundwater supplies, from toxic pollutants that may seep through the soil into aquifers and (iii) protect surface waters from being contaminated with agricultural chemicals such as fertilizers and pesticides, to enter in the food chain.

Since the publication of the renowned book of C.S. Piper entitled "Soil and Plant Analysis" in 1942 [5] a huge number of publications including books, book chapters and articles have been published about soil analysis. Soils are analyzed for a variety of reasons and purposes, for either diagnostic or prognostic applications. Testing of soils includes a series of analysis made to determine nutrient content, composition and other parameters for characterization of soil and to perform corrective actions if needed. This analysis can provide useful information in the context of sustainable development in order to protect the soil against multiple hazards, among them contamination, particularly that from human actions [6].

The soil quality assessment requires the analysis of many parameters. It implies the use of different conventional methods, generally based on the use of selective electrodes for pH [7], electrical resistivity, electromagnetic induction or coulterbased sensors for electrical conductivity measurements [8], loss-of-ignition and gravimetric methods for organic matter [9] gasometric and volumetric methods for calcium carbonate [10,11] as well as methods commonly involving wet digestion of solid samples in hot concentrated acids followed by inductively coupled plasma (ICP), mass spectrometry and optical emission or atomic absorption spectrometry (AAS) for trace element determination [12,13]. Hence, although it is technically possible to perform a wide range of analyses and derive from these data a soil fertility or health index [14], most of the required analyses are expensive, tedious, complex and highly time-consuming, which in practice makes it quite difficult to characterize the soil properties of a big area with the required spatial and/or temporal resolution and also without environmental deleterious side effects.

Soil and sediment analysis involves many analytical steps, as indicated in Fig. 2, from the sampling step to the sample conditioning and transport and laboratory operations. Through all these steps, there are many potential risks that could affect the environment and the quality of obtained data and, thus, a strong reduction in the number of steps and a faster analysis as possible is mandatory for improving the main and green analytical figures of merit.

In general, it is well accepted that air and water sample preservation and transport create serious drawbacks. However, it is also true in the case of soil and sediments which must be well conditioned to their transport to the laboratory and, thus, in situ analysis techniques, based on electrochemical and spectroscopy methods and the use of portable instrumentation, considered vanguard analytical tools [15], could provide a direct way for signal acquisition and treatment. This techniques are extremely useful tools for an early environmental diagnostic and to reduce the number and amount of samples to be transported to the laboratory.

In short, the need for fast and cheap methods that would enable the analysis of a big number of samples has been stressed in numerous studies [16] and vibrational spectroscopy has long been recognized as one of the most promising techniques [17].

2. Soil constituents and parameters

The components and parameters most usually studied by vibrational spectroscopy in soils include organic carbon content,

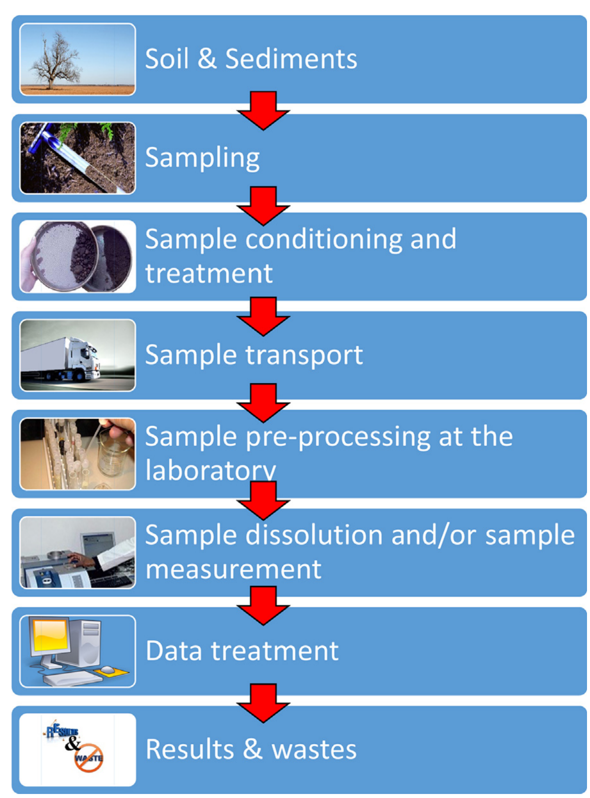

Fig. 2. Steps involved in soil and sediment analysis.