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NANOMATERIALS IN SOIL AND FOOD ANALYSIS

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Synonyms

Nanomaterials application in soil and food testing

Definition

Nanomaterials: generally referring to materials with the size of 0.1–100 nm.
Carbon nanotube: allotropes of carbon with a cylindrical nanostructure.
Biosensor: a device for the detection of an analyte that combines a biological component with a physicochemical detector component.

Introduction

The Food and Agriculture Organization (FAO) is the main United Nations agency specializing in all aspects of food quality and safety, and in all the different stages of food production, harvest, postharvest handling, storage, transport, processing, and distribution. Food analysis is the discipline dealing with the development, application, and study of analytical procedures for characterizing the properties of foods (Nielsen, 2003). These analytical procedures are used to provide information about a wide variety of different characteristics of foods, including their composition, structure, physicochemical properties, and sensory attributes. This information is critical to our rational understanding of the factors that determine the properties of foods, as well as to our ability to economically produce foods that are consistently safe, nutritious, and desirable and for consumers to make informed choices about their diet. One of the most important reasons for analyzing foods from both the consumers and the manufacturers' standpoint is to ensure that they are safe.

Precision farming has been a long-desired goal to maximize output (i.e., crop yields) while minimizing input (i.e., fertilizers, pesticides, and herbicides) through monitoring environmental variables and applying targeted action. A soil analysis is used to determine the level of nutrients found in a soil sample. Quality crops with high yields require a sufficient supply and maintenance of nutrient elements. As nutrients are utilized by one crop and not replaced for subsequent crop production, yields will decrease accordingly. Accurate monitoring of nutrient before and after crop production and soil analysis results will help the efficient management of fertilizer applications. Soil analysis can also help to reduce agricultural waste and thus keep environmental pollution to a minimum. Researchers are exploring to come up with sensors for detection of soil nutrients, pesticides, pollutants up to very minute fractions by exploiting novel properties of nanomaterials.

The definition of nanomaterial is based on the prefix "nano," which is from the Greek word meaning "dwarf." The word nanomaterials is generally used when referring to materials with the size of 0.1–100 nm; however, it is also inherent that these materials should display different properties from bulk (or micrometric and larger) materials as a result of their size (Rao et al., 2004). These differences include physical strength, chemical reactivity, electrical conductance, magnetism, and optical effects. The potential of nanomaterials to revolutionize the health care, textile, materials, information and communication technology, and energy sectors has been well publicized. In fact, several products enabled by nanomaterials are already in the market, such as antibacterial dressings, transparent sunscreen lotions, stain-resistant fabrics, scratch-free paints for cars, and self-cleaning windows.

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Nanomaterials such as nanotubes (NTs), nanowires (NWs), and nanoparticles present new opportunities as sensing platforms for biological and environmental applications. Having micrometer-scale lengths and nanometer-scale diameters, NTs and NWs can be manipulated with current microfabrication, as well as self-assembly techniques to fabricate nanoscale devices and sensors (Rao et al., 2004). Examples of different nanomaterials-based analytical techniques for the detection of major families of environmental pollutants, i.e., organic contaminants, heavy metals, and air pollutants are reported. Application of the nanomaterials in the field of soil and food analysis is promising. This article covers the recent developments and issues in electrochemical biosensors for food analysis such as ease of preparation, robustness, sensitivity, and realizations of mass production of the detection strategies. This article also emphasizes the current development of electrochemical biosensors combined with nanotechnology.

The synthesis, characterization, and utilization of nanomaterials are part of an emerging and rapidly growing field. Nanomaterials may be grouped under nanoparticles (the building blocks), nano-intermediates, and nanocomposites. Nanostructured materials are synthesized by supramolecular chemistry yielding nanoassemblies (Rao et al., 2004). The nanoparticles serve as the building blocks of nanomaterials and devices. They include nanocrystalline materials such as ceramic, metal and metal oxide nanoparticles; fullerenes, nanotubes, nanorods, and related structures; nanofibers and wires, and precise organic as well as hybrid organic–inorganic nanoarchitechtures such as dendrimers and polyhedral silsesquioxanes, liposomes, or nanosomes, respectively.

Nanocrystalline materials

Included here are ceramics, metals, and metal oxide nanoparticles. These materials are assembled from nanometer-sized building blocks, mostly crystallites. The building blocks may differ in their atomic structure, crystallographic orientation, or chemical composition. In other words, materials assembled of nanometer-sized building blocks are microstructurally heterogeneous, consisting of the building blocks (e.g., crystallites) and the regions between adjacent building blocks (e.g., grain boundaries). One of the primary applications of metals in chemistry is their use as heterogeneous catalysts in a variety of reactions (Rao et al., 2004). Due to their vastly increased surface area over macroscale materials, nanometals and oxides are ultrahigh activity catalysts. Nanometals and oxides are also widely used in the formation of nanocomposites. Aside from their synthetic utility, they have many useful and unique magnetic, electric, and optical properties.

Carbon nanotubes

Carbon nanotubes (CNTs) are hollow cylinders of carbon atoms. Their appearance is that of rolled tubes of graphite such that their walls are hexagonal carbon rings and are often formed in large bundles. Generally speaking, there are two types of CNTs: single-walled carbon nanotubes (SWCNTs) and multi-walled carbon nanotubes (MWCNTs) (Rao et al., 2004). As their names imply, SWCNTs consist of a single, cylindrical graphene layer, whereas MWCNTs consist of multiple graphene layers telescoped about one another. CNT-based nanodevices are a hot research area at the moment. Applications could include novel semiconducting devices, chemical sensors, and ultrasensitive electromechanical sensors (Wang, 2005).

Nanocomposites

Nanocomposites are materials with a nanoscale structure that improve the macroscopic properties of products. Typically, nanocomposites are clay, polymer or carbon, or a combination of these materials with nanoparticle building blocks. Nanocomposites, materials with nanoscale separation of phases can generally be divided into two types: multilayer structures and inorganic/organic composites. Multilayer structures are typically formed by gas phase deposition or from the self-assembly of monolayers. Inorganic/organic composites can be formed by sol–gel techniques, bridging between clusters (as in silsequioxanes), or by coating nanoparticles, in polymer layers for example.

Biosensors

Biosensors are molecular sensors that combine a biological recognition mechanism with a physical transduction technique. They provide a new class of inexpensive, portable instrument that permit sophisticated analytical measurements to be undertaken rapidly at decentralized locations. The sampling component of a biosensor contains a bio-sensitive layer that can either contain bioreceptors or be made of bioreceptors covalently attached to the transducer. The interaction of the analyte with the bioreceptor is designed to produce an effect measured by the transducer, which converts the information into a measurable effect, for example, an electrical signal. There are four major types of transducers: electrochemical (electrodes), mass (piezoelectric crystals or surface acoustic wave devices), optical (optrodes) and thermal (thermistors or heat-sensitive sensors). Among the various types of biosensors, the electrochemical biosensors are the most common as a result of numerous advances leading to their well-understood biointeraction and detection process (Eggins, 2002).

The state of the art of nanomaterials and nanotechnologies represents a new trend in the development of sensors and electronic chips that will have a big impact on the future of nanoscience. It is essential to distinguish between nanotechnology and nanomaterials, because in the first case nanotechnologies represent new possibilities for sensor construction and for the developing of novel methods. In the second case, nanomaterials have been widely used to immobilize enzymes, antigens, and nucleic acids on transducer surfaces, to promote the direct electron transfer reactions, and to amplify and orient the analytic signal of the bio-recognition events.

Applications

In chromatography

Separation science, based on chromatographic and electrophoretic techniques, has achieved many advances employing nanomaterials. Separation media and channels in the above two approaches have sizes and shapes comparable to those of nanomaterials, which makes the latter useful for specific applications in separation science on a micro- and nanometer scale. Nanomaterials have played various roles (e.g., modifier, stabilizer, and stationary phase) in chromatography. The effective pi–pi interactions between fullerenes and phenyl group have utilized to develop fullerene-based stationary phases for the separation of solutes with phenyl moieties in their structures. The conjugated pi- electron system on the surface of SWCNT as well as surface functionalization provides an opportunity to synthesize a stationary phase with good selectivity (Zhang et al., 2006). Nanoparticles, including silica nanoparticles, gold nanoparticles, titanium oxide nanoparticles, polymer nanoparticles, molecularly imprinted polymers, molecular micelles, and dendrimers, used as pseudostationary phases in CEC, have been reviewed by Nilsson et al. (2006).

In optical sensors

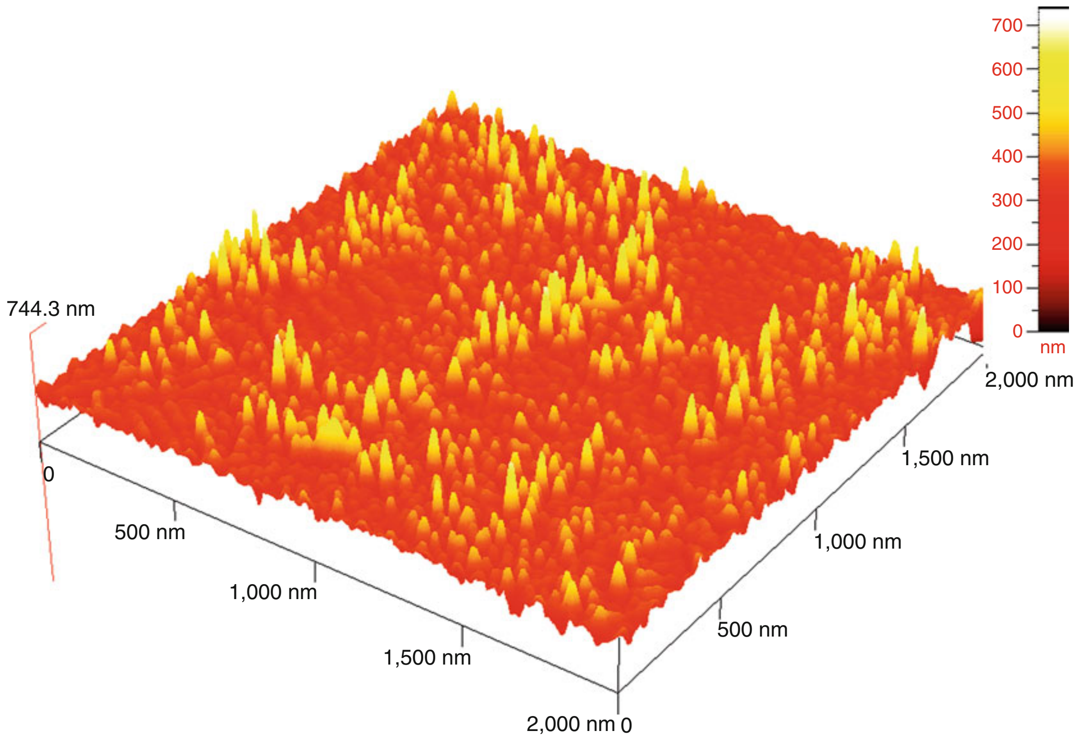
Nanomaterials-based optical sensors have been much interested to the trace detection of analytes of interest in the agriculture and food industry. The changes in the optical properties of nanomaterials such spectral absorbance, photoluminescence (PL), and chemiluminescence (CL) phenomena induced by the interaction between nanomaterials and various analytes is utilized to the determination of chemical and biochemical analytes (Shi et al., 2004). Quantum dots (QDs) are nanocrystals of inorganic semiconductors that are somewhat restricted to a spherical shape of around 2–8 nm diameter (Smith and Nie, 2004). Their fluorescent properties are size-dependent and therefore they can be tuned to emit at desired wavelengths (between 400 and 2,000 nm) if synthesized in different composition and size. In this way, QDs of different sizes can be excited with a single wavelength and emission controlled at different wavelengths, thus providing for simultaneous detection. These, together with their highly robust emission properties, make them more advantageous for labeling and optical detection than conventional organic dyes (Patolsky et al., 2006). Their high quantum yields and their narrow emission bands produce sharper colors, lead to higher sensitivity and the possibility of multiplexing of analysis (Tully et al., 2006). The unique optical properties of plasmonic nanoparticles have led to the development of label-free chemical and environmental sensor since the surface plasmon resonance (SPR) is sensitive to the local environment. Some research groups are exploring biosensors based on the SPR exhibited by metal nanoparticles (Haes and Van Duyne, 2002).

In electrochemical biosensors

One-dimensional (1-D) nanostructures, such as CNT and semiconductor- or conducting polymer nanowires, are particularly attractive materials for working electrode in biosensors. Nature of biosensing surface is very important, namely, the prolonged use of the sensor and an anticipated extended storage and working stability. High surface-to-volume ratio and electron transport properties of CNT opens the possibility of developing superior electrochemical sensing devices, ranging from amperometric enzyme electrodes to label-free DNA hybridization biosensors (Zhang et al., 2009). The possibility of direct electron-transfer between enzymes and electrode surfaces could pave the way for superior reagentless biosensing devices, as it obviates the need for co-substrates or mediators and allows efficient transduction of the bio-recognition event. “Trees” of aligned CNT in the nanoforest, prepared by self-assembly, can act as molecular wires to allow electrical communication between the underlying electrode and redox proteins covalently attached to the ends of the SWCNT (Gooding et al., 2003). Viswanathan et al. (2009) demonstrated that vertically aligned SWCNT on gold electrode for pesticides determination (Figure 1). Arrays of nanoscopic gold tubes or wires have been prepared by electroless deposition of the metal within the pores of polycarbonate particle track-etched membranes (Marc and Sophie, 2003). A sensitive and selective genomagnetic assay for the electrochemical detection of food pathogens based on in situ DNA amplification with magnetic primers reported by Lermo et al. (2007). Liposomes are microscopic, fluid-filled, pouches with endless walls that are made of layers of phospholipids identical to the phospholipids that make up cell membranes. Electroactive marker encapsulated immuno liposomes are typically used as signal amplifier for electrochemical immunoassays (Viswanathan et al., 2006). Chitosan (CS) is the second abundant polysaccharide and a cationic polyelectrolyte present in nature. Chitosan nanoparticles are promising biometarials for various analytical applications. Ferrocene-conjugated chitosan nanoparticles were used as the electroactive indicator of hybridization (Kerman et al., 2008).

Electronic tongue

Electronic tongue systems are hybrid micro or nanoarrays of electronic sensors that measure and compare tastes. E tongue is mainly based on potentiometric, voltammetric, ion-selective field-effect transistor (ISFET), piezoelectric, and optical sensors with pattern recognition tools for data processing. The information given by each sensor is complementary and the combination of all sensors results generates a unique fingerprint. Most of the detection thresholds of sensors are similar or better than those of



Nanomaterials in Soil and Food Analysis, Figure 1 Atomic force microscopic image of ssDNA-wrapped single-walled carbon nanotube (SWCNT) self-assembled monolayer on Au(111) surface (Viswanathan et al., 2009).

human receptors. The electronic tongue appeared to be capable of distinguishing between different sorts of beverages: natural and artificial mineral waters, individual and commercial brands of coffee, flesh food, and commercial and experimental samples of soft drinks containing different sweeteners (Scampicchio et al., 2008). Ciosek and Wroblewski (2007) have reviewed about recent developments of multisensor array based electronic tongue for food and soil analysis.

Electronic nose

Electronic nose is a specific kind of semiconducting sensor arrays that can mimic the natural olfaction sense, according to the electronic response (e.g., voltage, resistance, conductivity) arising from the different gas sensors, usually metal-oxide chemosensors. After exposure of the volatile compounds to the sensor array, a signal pattern is collected and results are evaluated with multivariate analysis or processed by an artificial neural network. Arrays of these nanosensors are able to detect molecules on the order of one part per million, sniffing molecules out of the air or taste them in liquid, suggesting applications in foods and food industry. A novel hybrid chemical sensor array composed of individual In_2O_3 nanowires, SnO_2 nanowires, ZnO nanowires, and single-walled carbon nanotubes with integrated micromachined hotplates for sensitive gas discrimination was demonstrated by Chen et al. (2009). Mycotoxins are secondary metabolites that mold produce naturally from some fungal species. Many researchers have reported efficient e-nose application such as mycotoxins analysis in grains (Falasconi et al., 2005), Salmonella typhimurium in stored beef (Zhang et al. 2008).

Mass-sensitive sensors

Researchers have taken advantage of the unique coupled semiconducting and piezoelectric properties of metal oxide nanowires to create a new class of electronic components and devices that could provide the foundation for a broad range of sensor applications. Plata et al. (2008) reported the microcantilever-based sensor for the determination of total carbonate in soil.

Conclusions

Soil and food analysis has become a very important and interesting area of research because of the rapid expansion of food trade and awareness of organic farming. Quality food is important both for consumer protection and also for the food industry. Nanomaterials such as nanoparticles, nanowires, and nanotubes open a new door as sensing platforms for sensor applications. They have allowed introducing novel strategies in sensors and biosensor technology. In particular, the development and application of nanomaterials in soil and food analysis are discussed, with focus on sensors, separation and extraction techniques, including the use of nanomaterials as transducer elements for sensors. Although not fully implemented yet, tiny sensors and monitoring systems enabled by nanotechnology will have a large impact on future precision farming methodologies. The prediction is that nanotechnology will transform the entire food industry, changing the way food is produced, processed, packaged, transported, and consumed.

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Cross-references

Agrophysical Objects (Soils, Plants, Agricultural Products, and Foods)
Chemical Imaging in Agriculture
DNA in Soils: Mobility by Capillarity
Electrochemical Measurements in Soils
Enzymes in Soils
Leaching of Chemicals in Relation to Soil Structure
Oxidation–Reduction Reactions in the Environment
Physical Degradation of Soils, Risks and Threats
Precision Agriculture: Proximal Soil Sensing
Quality of Agricultural Products in Relation to Physical Conditions

NATURE CONSERVATION MANAGEMENT

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Synonyms

Biological resources management

Definition

Nature conservation management (NCM) is a system of actions aimed at permanent conservation and sustainable use of the resources and values of the natural environment.

The main elements of NCM system

The growing scale of anthropogenic transformation of the environment causes that NCM is becoming an increasingly important field of human activity and requires higher and higher qualifications. At present, the NCM system (NCMS) comprises the integrated functioning of five subsystems (Chmielewski, 2007): (1) subsystem of diagnosis (DS); (2) planning subsystem (PS); (3) decision-taking subsystem (DTS); (4) subsystem of tasks realization (TRS); (5) certificate and control subsystem (CCS).

(1) For rational management of nature conservation we must first acquire knowledge about the functioning of natural ecosystems and about their responses to various human actions (Pullin, 2007; Wu and Hobbs, 2007). Organization for economic co-operation and development (OECD) presents the organization of the system of natural environment diagnosis as the following sequence: Drivers – Pressures – State – Impact – Response, referred to by the abbreviation DPSIR model (Watt and Young, 2007). **Driving forces** are anthropic activities and processes that cause pressures production (agriculture, industry, transport, etc.), consumption, recreation, etc. **Pressures** are described as direct stress from the anthropic system on the natural environment: release of polluting substances, radiation emissions, use of soil, intake of natural resources, and other changes of the natural environment. **State** – means conditions and tendencies in the natural environment, air, water and soil quality, global temperature, loss of biodiversity, etc. The description of the state of the environment is not easy: it should comprise at least four stages: (a) retrospection, that is, analysis of changes that have taken place in the environment over the last several decades; (b) inventory of nature resources; (c) valuation of nature resources; and (d) analysis of the potential of the natural environment (Chmielewski, 2001). **Impacts** are effects on the anthropic system due to changes in the natural environment: negative consequences on human health, economic loss in production activities, floods, etc. **Responses** are actions of the anthropic system aimed at solving environmental problems (prevention, pollutants elimination, biodiversity conservation, ecosystem restoration, ecological compensation, etc.) (Fiedler and Jain, 1992). The "**Responses**" element, however, is not a typical element of the diagnostic system as it comprises elements of three further subsystems of the NCMS (2–4).

(2) The results of diagnosis of the state of the natural environment constitute the basis for initiating the planning subsystem, the main element of which are *nature management plans* (or nature conservation plans) for the most valuable areas: national parks, nature reserves, Natura 2000 sites, landscape parks, etc., as well as the *sustainable development strategies* and *local development plans* for the various levels of hierarchy of administrative organization of the country. Nature management plans are mostly worked out by the governmental nature conservation services; however, in the process of their preparation local government representatives take part as well. Achievement of compatibility and agreement of the provisions of the nature conservation plans with the local development plans are of key importance for smooth management of resources of the natural environment.

(3) On the basis of these two types of plans, the administrative decisions concerning nature conservation actions as well as land-use changes, housing and road construction, development of services, and other activities are undertaken. They may pertain, for example, to water damming, stand reconstruction, moor plant succession control, but also to the architecture style of buildings, tourist facilities, and creating tourist routes and educational paths. All administrative decision should contain relevant provisions concerning the conservation of natural values, sustainable utilization of nature resources, and harmonious scenic beauty design. Unfortunately, many decisions – particularly those concerning new economic investments, neglect the ecological conditions or marginalize them.

(4) and (5) Observance of the provisions contained in administrative decisions is of fundamental importance for nature conservation and landscape quality. This purpose is served by a system of certification, control, standards, and indexes of quality of the environment (Keulartz and Leistra, 2008; Schmidt et al., 2008). However, losses observed in the resources and values of the natural environment indicate that in many regions that system is not effective. For a better nature conservation management it is necessary to develop urgently a network of biodiversity and landscape diversity monitoring as well as urban monitoring. It is also necessary to systemize the gathering of these data, by a common introduction of Spatial Information Systems based on advanced computing technologies. Such systems are one of the key instruments facilitating effective protection and sustainable management of resources and unique natural values areas on the world scale.

Key instruments for effective functioning of the five subsystems of NCMS

Each of the five subsystems of the NCMS has at its disposal specialist instruments that should ensure its effective functioning. Of key importance for the subsystem of diagnosing, the state of the natural environment is the financing and organization of research and of the network of monitoring of the natural environment. For better understanding of the functioning of nature and for the purpose of development of effective methods of nature resources management theories are constructed as well as models for conservation and wildlife management (Samson and

Knopf, 1996; Harris, 2007). For the quality of the planning subsystem, of fundamental importance is the legal system, the quality of education of landscape ecologists, landscape architects, space planners and engineers, as well as the operating conditions of design companies and offices. The quality of administrative decisions depends primarily on the quality of the relevant legislation and on the level of professionalism of administration officers and on the quality of internal audit. In the process of realization of the plans and decisions, that is, in the course of the practical utilization of nature resources, highly important is the ecological policy of the particular countries, their legal systems, ecological education of the people, education of the administrative cadre, organization of the system of certification and audit. At all levels of organization and at all stages of implementation an important instrument of the NCMS should be the cost-effectiveness analysis, permitting to identify which NCM methods and techniques should be applied for the invested funds and undertaken organization activities to bring the best ecological effects (Wätzold, 2005).

Conclusion

NCM is becoming a more and more extensive and highly specialist branch of knowledge and a broader and broader forum of practical activity. The NCM system has an extensive infrastructure and numerous instruments that should ensure its effective operation. In spite of all this, we are still witnessing many processes unfavorable for nature, such as the shrinking of the ecological space, landscape structure fragmentation, and loss of biodiversity. These challenges necessitate further intensive work on the ecological education of the society and on the development of the NCM system at the level of regions, countries, continents, and the whole biosphere.

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Cross-references

Climate Change: Environmental Effects
Monitoring Physical Conditions in Agriculture and Environment
Wetlands, Management, Degradation and Restoration

NEURAL NETWORKS IN AGROPHYSICS

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Synonyms

Artificial Intelligence; Artificial Neural Network; Neural Network

Definition

Artificial neural network (ANN) – a mathematical model, based on the calculations made by the network of interconnected artificial neurons or perceptrons. Neural networks are a subclass of wider range of calculation techniques called *soft learning techniques*.

Introduction

First ideas concerning artificial neural networks are dated back to 1940s, when for the first time model of an artificial neuron was formulated (McCulloch and Pitts, 1943) and basic methods of neural networks training was developed (Hebb, 1949). Further theoretical developments and first practical applications of neural networks took place in 1950s and 1960s. The first image classification system was built (Rosenblatt, 1958). A new effective method of network learning-supervised training was developed (Widrow and Hoff, 1960). The multipurpose neural networks ADALINE and MADALINE, used for weather forecasting, in adapting control systems, and for image recognition, was built (Widrow, 1962). After initial period of rapid developments, works on neural networks stagnated some, until 1980s, when performance of computational systems increased enough, to allow for new ANN applications. New types of neural networks were discovered and a new type of training algorithm was developed (Hopfield, 1982; Kohonen, 1984). From 1980s period of rapid theoretical developments and increasing practical applications started.

Nowadays artificial neural networks emerged into one of the wider used soft learning techniques. The artificial neural networks are used in scientific developments and in wide range of practical applications. Many agrophysical objects and processes may be modeled by artificial neural networks.

Basic concepts of neural networks

Artificial neural networks are mathematical models which allows for data processing or information storage. These mathematical models consist of neural network themselves and algorithms or methods for neural network training and evaluation of its performance. Concept of artificial neural network was taken from organization of biological brain. Neural network is a set of interconnected artificial neurons and links between them.

Artificial neurons, called also in ANN nomenclature a perceptron, have properties similar to real brain's biological neuron. It has many inputs, called *dendrites*, and only one output – *axon*. In fact, behavior of the perceptron is modeled by simple nonlinear function of the form Equation 1:

$$y = f_{\mathrm{act}}\left(w_0 + \sum_{i=0}^{n} w_i x_i\right) \tag{1}$$

where y – is an output signal from neuron considered, x_i – are input signals from other neurons, w_i – are weights specific for i-th dendrite of artificial neuron, w_0 – is a constant bias signal used in many neural networks types (called also inhibitory input), finally f_{act} – is a so called activation function. Based on this equation, the output of each neuron is simply a weighted sum of input signals, processed by additional activation function.

There are many types of activation functions used in ANN developments. Some of them commonly used are grouped in Table 1.

In neural networks, output from one neuron is connected to inputs of other neurons. This net of interconnected neurons has parallel data processing capabilities, and may be used to store the information.

There are many neural networks topologies, but in agrophysical research two of them are commonly used. For applications based on evaluation of the output, based on input variables, multilayer neural networks are used.

Neural Networks in Agrophysics, Table 1 Sample activation functions

Binary (0,1)	Log-sigmoid	Hyperbolic	Linear
$f_{\mathrm{act}}(z) = \begin{cases} 0, & z < 0 \\ 1, & z \geq 0 \end{cases}$	$f_{\mathrm{act}}(z) = \frac{1}{1 - e^{-z}}$	$f_{\mathrm{act}}(z) = \frac{e^z - e^{-z}}{e^z - e^{-z}}$	$f_{\mathrm{act}}(z) = z$

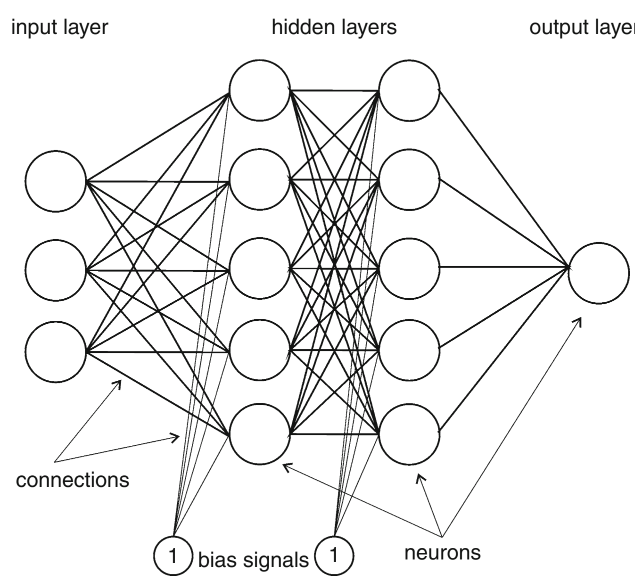
These neural networks are mainly feedforward neural networks, but some applications utilize feedback neural networks also. If modeled problem is based on some kind of classification, self-organizing map (SOM) neural networks are typically used.

The wider range of applications uses single layer or multilayer feedforward network. Such network has layered architecture, see Figure 1. The first neuron layer consists of input neurons. These neurons are used to enter processed data into the network. Following input layer are one or more hidden layers. The last is the output layer, values of neurons from this layer represent results generated by neural network for specific input values. Outputs of neurons in feedforward networks from one layer are connected to inputs of neurons in the next layer. This allows for trained network to evaluate its output for input variables.

Common feature of feedback neural networks is its recurrence. Due to this, outputs of neurons from one layer are connected to input of the same layer. This kind of neural network may be used for modeling of processes, because of calculated output values changes for each subsequent evaluation.

Training of the neural networks

Neural network consists of neurons and weights describing connections between neurons. While number and type of neurons for specific neural network is fixed, weights for each connection may be changed. Processes of adjustment of weight values have a crucial role for applications of neural networks, and it is called neural network training. There are many algorithms/methods used for ANN training. Generally each neural network topology has specific



Neural Networks in Agrophysics, Figure 1 Feedforward neural network.

training method. Training methods may be generalized into two categories: supervised training and unsupervised training.

In most of agrophysical applications, where feedforward or feedback neural networks are used, proper method of network training is some kind of supervised training technique. Supervised training assumes knowledge of proper output responses for set of inputs. The origin of this dataset is application dependent, but the most frequent source of training data is some kind of experiment, survey, or measurement. The basic idea of supervised neural network training is to compare results/outputs generated by neural network for inputs, for which proper output values are known. Based on difference between evaluated by network output results and known outputs from training dataset, called training error, weights of neural network are subsequently adjusted.

Data which are used for learning neural network are commonly divided into two disjointed datasets: training dataset and testing dataset. Training dataset is used for training of the neural network, while on the testing dataset performance of trained neural network is evaluated. The aim of neural network training is to adjust neural network weights in such way that error for testing dataset, called test error, will be minimal. The smaller the test error is, the better generalization properties the neural network has, and will better perform for new, unknown input data.

Presentation of training data to the network and weight adjustments are repeated many times, until neural network performs well. Generally, training error decreases in subsequent neural network training procedure repetitions. However testing error, which is the criterion for neural network evaluation, in some circumstances, may remain at constant level, or even grow up slightly after initial decrease. This phenomenon is known as over learning that occurs especially when training dataset is too small in comparison to number of neurons in the neural network. When over learning happens, testing error increases for subsequent steps of learning, while training error decreases.

Agrophysical applications

Basic tool for scientific development utilizing artificial neural networks methodology is appropriate software. There are many commercially and freely software packages available. Beside many others, some freely available software is worth to mention: SNNS (Zell et al., 1995) and its successor JavaNNS. EMERGENT (Aisa et al., 2008), and program R (R Development Core Team, 2010) with appropriate modules are free multiplatform neural network solutions.

Neural networks may be used in many fields of agrophysical developments. Typical applications include: modeling of transport processes in the soil medium, modeling of hydrophysical properties of soils, soil classification based on different criteria, crop production modeling, or food quality evaluation. These applications of neural networks can be generalized into two categories: problems based on prediction of some property and problems based on some kind of classification.

Soil science

One of the fields where neural networks are extensively used is pedotransfer functions (PTF) development. Pedotransfer functions are mathematical models, which allow for approximating difficult measurable soil parameters, based on some easily measurable input information. Typically, soil water retention curve and hydraulic conductivity of soils are evaluated by PTFs. For PTF development many techniques may be used (Wösten et al., 2001), from legacy regression models (Walczak et al., 2006) to neural networks and beyond (Lamorski et al., 2008).

For PTFs development feed forward neural networks are used, as these applications are based on approximation. Typically among others input parameters for PTFs evaluating retention curve are: particle size distribution, soil porosity, bulk density, and organic carbon content. Some PTF models use as input parameter measured water content for one specific value of water potential. The output of neural network is a retention curve approximation. There are numerous models used for evaluating soil water retention curve, which may be divided into two classes: models which evaluate water content for selected values of water potential (Lamorski et al., 2008; Pachepsky et al., 1995) and models which evaluate parameters of some kind of retention curve approximation function, mainly in the form of Mualem and van Genuchten approximation (Schaap and Leij, 1998; Minasny and McBratney, 2002).

The other usage of ANN to evaluation of hydrological properties of soils are PTFs for soil hydraulic conductivity approximation. Soil hydraulic conductivity is one of parameters which influences soil water transport phenomena. For many purposes approximations of value of hydraulic conductivity may be used instead of measured values. One of the method, which may be used for soil hydraulic conductivity approximation, is to use neural network modeling. This approach includes models for saturated hydraulic conductivity evaluation (Merdun et al., 2006; Schaap et al., 1998). Unsaturated soil hydraulic conductivity may be approximated by neural networks also (Schaap and Leij, 2000).

Soil classification is the other application of ANN to soil science. One of the commonly used soil classification systems are texture based classification systems. They allow for determination to which class soil belongs, based on its granulometric distribution. For other purposes, different classification criteria than soil texture may be used. The common problem in soil classification systems is that one wants to determine some kind of qualitative in nature soil parameter. In soil surveys such parameters evaluation are made by properly trained and experienced researcher. It is not easy task to map such soil features from a set of quantitative, easily measurable soil parameters, but there are attempts to build such expert systems. One of important soil properties is its aggregation structure. Soil aggregation is a qualitative parameter which cannot be directly connected to soil quantitative parameters. Although there were attempts to classify soil to one of three aggregate classes (granular, blocky or massive) based on soil granulometric composition and organic carbon content using feed forward neural networks (Levine et al., 1996).

Crop production and food quality

The other field of investigations where artificial neural networks are used is crop production, especially with precision agriculture relying on advanced monitoring, measurement (Precision Agriculture: Proximal Soil Sensing) and modeling techniques. Fertilization is one of the key practices used in crop production, proper dosage of fertilizer, appropriate for current field conditions may be determined by neural networks (Yu et al., 2010). Prediction of crop growth is another example of usage of neural network. There are ANN models which allow for crop yield prediction based on some input parameters (Green et al., 2007). Irrigation is a common agricultural technique. Effective usage of water is an important objective; artificial neural networks may be also used in optimization of water usage (Morimoto et al., 2007). Food quality is very important and may be influenced by many external factors, during crop harvesting, storage, and processing. Some properties of crops important for food quality may be modeled by ANN. Example applications include method of estimation of sorption isotherm for rice (Amiri-Chayjan and Esna-Ashari, 2010), which is important factor influencing rice storage conditions and has impact on rice quality. Chemicals are commonly used in tillage practice, for crop fertilization, or protection against pests. Unfortunately, if inappropriately used, chemical compounds may accumulate in crops and influence quality of food produced. The key point is to prevent food contamination, by optimization of chemicals usage (Du et al., 2008). In some circumstances toxins may be introduced to food in naturally occurring phenomena. One of application of ANN allows for predicting contamination of peanuts by aflatoxin produced by naturally occurring mildew (Henderson et al., 2000) in dependence of plant growth conditions.

Modeling approaches

Processes occurring in agrophysical objects may be modeled using strict mathematical, physical, or chemical methodology. In such approach phenomena are modeled exactly. Although in some practical applications rigorous modeling methodology is not needed. Artificial neural networks are the tool which may be used in such circumstances. The main idea of learning based modeling is to build and train ANN which will predict approximated values, based on previously registered values. Forecasting neural networks may be used for modeling wide range of agrophysical processes. Possible applications include forecasting of soil moisture, soil temperature, or contaminant concentration. There is a known model (Raju, 2001) utilizing ANN to evaluate soil temperature and evaporation, based on air relative humidity, wind speed, and air temperature. The other study (Han and Felker, 1997) describes method of estimation daily soil water evaporation, where neural network input factors are: air humidity, air temperature, wind speed, and soil water content. Soil moisture predictions are also possible (Liu et al., 2008), neural network was used for prediction of future soil moisture at specified depth, based on previous values of soil moisture readings from the same depth. Also they are successfully used for modeling of post-harvest drying process (Neural Networks in the Modeling of Drying Processes).

Summary

Proper description of processes occurring in the soil–plant–atmosphere continuum has a crucial role in agrophysical development. Artificial neural networks are useful for a range of agrophysical applications, including estimates of soil water retention, movement, evaporation, temperature, crop growth, post-harvest drying process, and food quality. ANN descriptions are particularly useful when strict measurement or modeling methods cannot be used.

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Cross-references

Agrophysical Objects (Soils, Plants, Agricultural Products, and Foods)
Databases on Physical Properties of Plants and Agricultural Products
Databases of Soil Physical and Hydraulic Properties
Hydraulic Properties of Unsaturated Soils
Hydropedological Processes in Soils
Neural Networks in the Modeling of Drying Processes
Pedotransfer Functions
Physical Phenomena and Properties Important for Storage of Agricultural Products
Physical Properties as Indicators of Food Quality
Precision Agriculture: Proximal Soil Sensing

NEURAL NETWORKS IN THE MODELING OF DRYING PROCESSES

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Synonyms

Artificial intelligence modeling

Definition

Neural network (NN) is an artificial intelligence method in order to determine the relationship between the moisture distribution in the material bed to be dried and the physical parameters of the drying air temperature, humidity, and airflow rate. During its application, an emphasis should be given on the selection aspects of neural network structure and specifically to the influencing parameters as sampling time, randomized training, different training algorithms, number of hidden neurons, number of linked data series, and type of validation data. A properly selected structure of neural network model can be used to determine the moisture distribution in the drying bed. It can also be stated that besides other factors the selection of training and validation input data for NN model has a strong influence on the applicability.

Introduction

Concerning the postharvest processes, besides the energy consumption impacts, the quality issues remain the most determining factor. The main problem in the grain drying process is to determine the moisture content in the material bed. Overdrying requires excessive energy and even can damage the quality of the dried material, especially in case of seed. On the other hand, the grain will be vulnerable to mildew if the moisture content remains high. There is an option to determine the moisture content in the drying bed by measurement but the accuracy of this approach is probably not satisfactory. Weather conditions and dust have a great effect on the accuracy, as well. Another way to determine the moisture distribution is to calculate the moisture content based on drying air parameters using physically based or black-box models. Physically based models give a moderately good result in most cases but it normally takes a great effort to identify their parameters and also to solve the model itself. Derivation of the classical black-box models seems to be an uncomplicated approach. However, the application of such models is mainly limited to process control.

The artificial neural network is a well-known tool for solving complex problems and it can give reasonable solutions even in extreme cases or in the event of technological faults (Lin and Lee, 1995). Huang and Mujumdar (1993) created a neural network in order to predict the performance of an industrial paper dryer. The neural network model by Jay and Oliver (1996) was used for predictive control. Trelea et al. (1997) successfully used explicit time and recurrent neural networks for modeling the moisture content of thin-layer (5 cm) corn during the drying process and for wet-milling quality at constant airflow rate and absolute humidity and variable temperature. Thyagarajan et al. (1997) modeled an air heater plant for a dryer using a neural network. Sreekanth et al. (1998) predicted psychometric parameters using various neural network models. Kaminski et al. (1998) used a neural network for data smoothing and for modeling material moisture content and temperature. The literature cited clearly encourages further study of the application of artificial neural networks to modeling of postharvest and within that the drying process. However, application of neural networks for drying processes takes a significant consideration to the influence of sampling time, randomized training, different training algorithms, number of hidden neurons, number of linked data series, and type of validation data. The structure of the NN is to be selected to include all the inputs and outputs of the drying system.

Modeling approaches

As a classical way of modeling, the physically based models (PBM) are normally used to determine the performance evaluation of drying process. However, the PHBs make some difficulties in setting up the most appropriate equations, to determine the accurate values of their parameters, and to find the most efficient methods for the solution. At the same time, there is a good option of the use of NN for modeling purposes along with their uncertainties and difficulties in determination their optimal topology and parameters for the given problem, for example, postharvest technology this time. Sometimes, in order to provide input data for training the neural network a well-identified physically based model are considered to use instead of full-scale or laboratory measurements.

Several NN topologies could be considered for the use of modeling the drying process as it was suggested by Farkas et al. (2000a). The choice of a topology depends on careful selection of the input system variables and the controlled output variables, for example, moisture contents in the different layers of the material bed. It should be stated that the selection of NN topology is an essential step.

Training the neural networks

Input data used for training the neural network of different structure should be the same. The drying air temperature, airflow, and absolute humidity have to be changed randomly to train higher order dynamics, as well. The outlet air temperature and absolute humidity in the layers could be calculated on the basis of an appropriate physically based model because of its difficulty in measurements. In each training loop, each data record can be trained, for example, with back-propagation algorithm (Lin and Lee, 1995). One training step means to calculate the error between the network output and the desired output and to modify the weight of the neural network. During the training process, all the introduced neural network structures have different training speed, for example, the number of calculation loops in order to reach the required accuracy. The cost function expresses the stop condition of the training. The selection of training input data for NN model has a strong influence on the applicability.

Validation the neural networks

For validation purposes, constant and multi-flow data are normally chosen because of the real industrial drying processes. The validation data for multi-flow dryer are taken from outside weather parameters. The airflow is switched between two states to simulate intermittent drying, the air temperature, and humidity considered based on weather condition. The selection of validation input data for NN model has a strong influence on the applicability. During the validation calculation beside the correlation coefficients the average and maximal deviation could be used to estimate the behavior of the neural network model.

Sensitivity of the neural networks

Extensive studies on validation of the NN model have been carried out along with the influences different parameters as the sampling time, the randomized training, the different training algorithms, the number of hidden neurons, the number of linked data series, and the type of the data as it was suggested by Farkas et al. (2000b). In this experiment, a three layer feed-forward neural network with six hidden neurons was used. The NN contained also delayed feedback from the output to the input.

It was found that increasing the time step decreases the average deviation between the original training points and the outputs of the NN. It can be observed that the fluctuations are larger at the beginning of the drying if small sampling time is selected, because of the large number of points. The explanation of this effect can be that the back-propagation algorithm minimizes the difference between one input–output training pair in one step, and then it modifies the network weights based on the calculation point by point. In such a way, the neural network partly "forgets" the behavior of the process at the beginning. The more points are used the higher fluctuation will be at the beginning of the process. Randomized training can be used for reducing this effect when the points are randomly selected to train the neural network.

In order to avoid high fluctuation at the beginning of the process, the training pairs are randomly selected from the entire drying period. Using randomized training pairs for back-propagation algorithm caused considerable improvement in the results even in case of a large number of training pairs. The result shows furthermore that there is no fluctuation effect at the beginning of drying process, so using randomized training pairs is to be recommended for real applications.

Preliminary studies showed that the original back-propagation algorithm could be slightly improved after some modifications. The first changing was to introduce an adaptive learning constant during the training. Another modification was changing the weights. After such experiments it can be concluded that there is almost no influence caused by the modifications, so it can be concluded that the original algorithm could be efficiently used without any modification.

A sensitivity study was performed in order to determine the influence of the number of hidden neurons in the NN. The sampling time was selected as 120 s along with randomized training pairs and the original back-propagation algorithm. From the results, it can be concluded that the best approximation was achieved when the number of hidden neurons was between 3 and 5. So the number of neurons in the hidden layer could be optimized in any special application cases.

As it was said before, it has been realized that a single data series is not reasonably enough for training the NN. Training with one data series, validation results can be unsatisfactory in case of changing in input data. To achieve better performance in neural network modeling it seems a good idea to link together different number of data series as one virtual drying process. The result shows that increasing the number of linked data series for training increases the accuracy of the NN model. Fast random signals caused the largest fluctuation at low number of linked data series.

There were several trials to validate the NN with different (constant, slow, and fast random) type of data. It can be observed that the case of slow random training gives reasonable good result for both constant and fast random validations. Constant training gives the worse result for the case of fast validation signal.

Summary

Neural network modeling is a reliable tool for determining the moisture and temperature distribution in the course of drying process. In order to set up an appropriate model, sufficient number of measurements should be available for training the neural network. The sensitivity aspect of the neural network model should be taken into account during the training and validation. Generally saying, the NN can be successfully applied especially for process control purposes.

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Cross-references

Drying of Agricultural Products
Grain Physics
Neural Networks in Agrophysics
Physical Phenomena and Properties Important for Storage of Agricultural Products
Physical Properties of Raw Materials and Agricultural Products
Quality of Agricultural Products in Relation to Physical Conditions
Rheology in Agricultural Products and Foods
Shrinkage and Swelling Phenomena in Agricultural Products
Solar Drying of Biological Materials

NITRIFICATION

The oxidation in biological process of ammonia to nitrate, via nitrite.

NONDESTRUCTIVE MEASUREMENTS IN FRUITS

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Synonyms

Nondestructive measurement of fruit quality

Definition

Technologies used to measure quality parameters in fruit of not destructive form.

Introduction

Nondestructive testing was, and still is, a priority research area for specialty crops; its aim is to assess or quantify product properties and characteristics for the purpose of quality and safety monitoring and control. Sensors have been widely recognized for their potential to identify product properties, and they have been translated into industrial technologies, as evidenced by thousands of engineering research publications during the past 50 years.

Fruit quality is related to both internal variables (firmness, sugar content, acid content, and internal defects) and external variables (shape, size, external defects, and damage). Increasing consumer demand for high-quality fruit has led to the development of optical, acoustic, and mechanical sensors that determine this quality (Nicolaï et al., 2006). Fruit packing companies need to measure these quality variables, but they need to do so in a nondestructive manner. Manufacturers and research groups have understood this complexity and are currently developing sensors with this aim.

The development of sensors to measure fruit internal and external quality variables on a nondestructive way is one of the challenges of postharvest technology. These include static and online sensors that use different technologies for determining fruit quality parameters. Although many techniques are under development, some companies already market instruments that determine the internal quality of fruit.

Internal fruit quality parameters

Fruit firmness

Fruit firmness is one of the most important quality variables; it is an indirect measurement of ripeness and its accurate assessment allows appropriate storage periods and optimum transport conditions to be established.

Traditionally, fruit firmness has been estimated in a destructive manner by means of the Magness Taylor test. This can be performed in the laboratory or with portable equipment, and is based on the introduction of a cylindrical head into the flesh of a peeled fruit to measure the maximum penetration force. Depending on the equipment used, other variables can be measured such as maximum force, deformation, and the values for different relationships between force and deformation. However, the Magness Taylor test has three main drawbacks: it is destructive, measurements are highly variable (by up to 30%), and it cannot be used in online situations. Nevertheless, this technique is well accepted and used for classifying fruit by many packing companies and quality laboratories.

Technical advances over the last few decades have led to the development of nondestructive devices capable of measuring fruit internal variables (Delwiche et al., 1996). Originally, these devices were developed for use in the laboratory, but have been adapted for online use (as have weight or diameter-measuring devices).

Fruit firmness can be estimated by different techniques including the measurement of variables extracted form force–deformation curves, the analysis of impact forces, the rebound technique, the measurement of acoustic responses to vibrations and impacts, the measurement of optical properties, and nuclear magnetic resonance (García-Ramos et al., 2005).

Sugar content, acid content, and internal defects

The interaction between light and fruit tissues can be used to measure fruit internal quality (Nicolaï et al., 2007). An optical sensor consists of a light source and a receiver that records the optical signal. The optical signal has different wavelengths. According to the light pathway inside the sample, there are two main optical techniques: reflectance (incident light penetrates the external tissues and exits toward the sensor near the entering point) and transmittance (incident light goes through the tissues and hits the sensor on the opposite side of the fruit – or at least 90° away from entrance point).

The technology more used is the near infrared reflectance spectroscopy (NIR). This technique, which measures the reflected spectrum of a sample lit with halogen light is closely related to that employed by optical equipment (e.g., cameras). Much research effort is currently being made in this area.

Commercial, online, optical devices based on NIR spectroscopy are available. Some devices were developed for use with melons but have been successfully used with pears, apples, peaches, and Sharon fruit. These sensors can handle 2–5 fruits/s depending on the species. The internal variables measured are sugar content plus an indirect measurement of firmness ("ripeness").

External fruit quality parameters

Shape and size

The estimation of the size and form of the fruit is realized by means vision systems in the range of the visible and near infrared spectrum (Moreda et al., 2009). Nevertheless, commercial vision systems do not yield in general the high precision volume estimates required for density sorting, because they compute volume from two-dimensional (2D) images. Nowadays, three-dimensional (3D) machine vision systems are beginning to be introduced in some food industries. This trend could eventually spread to fresh produce packinghouses, where 3D cameras could be used, apart from calculating accurate volume, shape sorting, and surface area.

Weight

Fruit weight estimation is commonly performed with an electronic weight sizer. These sensors are implemented in commercial fruit packing lines and can be recalibrated for different weight groups. The accuracy achieves ±1 g working at speeds of 1 m/s (until 10 fruits/s).

Color

Light in the visible region (approximately 400–780 nm) can provide color and/or pigment information about horticultural products. Skin color may be indicative of maturity for some horticultural products such as banana, mango, and tomato (Edan et al., 1997). However, for many other horticultural products, skin color is not a good and reliable indicator of their maturity/quality. Color more directly relates to product appearance, which is important to the consumer perception of product quality (Abbott, 1999). Hence, color vision technology is widely used in the horticultural industry to ensure consistent product items in size, shape, and color.

Summary

The increasing demand of fruit quality by consumers makes necessary the development of technology to achieve this goal. Most of the fruit packing lines already have equipments capable of quantifying the parameters of external quality of a fruit (size, weight, and color) in line and of not destructive form. During the recent years, the enterprises and research groups have developed technologies for the nondestructive measure of internal quality parameters (sugar content, acids content, firmness, etc.). These include static and online sensors that use different technologies for determining fruit quality parameters. Although many techniques are under development, some companies already market instruments that determine the internal quality of fruit.

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Cross-references

Agriculture and Food Machinery, Application of Physics for Improving
Color in Food Evaluation
Fruits, Mechanical Properties and Bruise Susceptibility
Machine Vision in Agriculture
Physical Properties as Indicators of Food Quality
Quality of Agricultural Products in Relation to Physical Conditions

NONDESTRUCTIVE MEASUREMENTS IN SOIL

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Definition

Nondestructive measurements in soil are a wide group of techniques used in science and agriculture and applying ground-installed sensors to evaluate the properties of soil without causing damage.

Nondestructive and destructive measurements

Contrary to destructive measurements in soil, where the original physical, chemical, or biological properties of the measured object cannot be recovered, in nondestructive testing the measured object can function correctly after the measurement process. For example, the standard thermogravimetric method for the measurement of soil volumetric water content is destructive, while TDR (time-domain reflectometry) method is nondestructive. In thermogravimetric method, the soil sample is permanently removed from its original location and during the process of drying its structure and biological components are destroyed. In TDR method, after one-time installation disturbance in a fixed location, repeated and automated measurements are allowed without causing any damage to any soil constituent.

Nondestructive measurements or tests should be distinguished from noninvasive ones, which include diagnostics, that is, procedures that do not involve tools breaking the soil structure (see *Noninvasive Quantification of 3D Pore Space Structures in Soils*) and the skin or physically enter the body (ultrasound, X-rays, endoscopes, computer tomography). The noninvasive measurements that do not use sensors installed in the soil include: NIRS (near infrared reflectance spectroscopy) for determination of soil texture and carbon content, airborne and satellite remote sensing for characterizing soils for plant available water capacity and topsoil properties (Schmidhalter et al., 2008), GPR (Ground Penetrating Radar), electromagnetic induction for collecting information about field heterogeneity of soil texture and soil water content, NIRS (near infrared spectroscopy) for determination of soil texture and carbon content. Their primary application is precision agriculture and site-specific soil treatment to achieve optimal plant production under sustainable agricultural and environmental conditions.

These methods usually require additional and traditional ground measurements for calibration purposes.

Nondestructive measurement techniques are commonly used in industry because they do not permanently alter the article being inspected saving both money and time in product evaluation, troubleshooting, and research.

Elements of nondestructive measurements in soil

Agrophysics as an applied and interdisciplinary science adopts nondestructive measurement techniques from other fields of science and industry. The fundamental elements for successful nondestructive measurements in soil apart from a sensor, usually working in the indirect measurement mode, are: data-logging features of the applied measurement equipment, battery supply (frequently supported by charging solar panel) powerful enough to work without replacement for at least one measurement season, and communication option (preferably wireless) to transmit measured data as well as the experiment configuration in both direction between the field location and the operator's computer. Table 1 presents the selection of the most popular nondestructive measurements in soil, which are used for the measurement of soil water status.

Nondestructive Measurements in Soil, Table 1 Selection of the most popular nondestructive and noninvasive soil water status measurements methods

Measurement method	Directly measured quantity, physical principle, soil property measured, and references	Remarks
TDR (time domain reflectometry)	Velocity of propagation of electromagnetic wave (step or needle pulse) along the metallic parallel or coaxial waveguide (TDR probe) fully inserted into the soil. It is very well correlated with the real part of the soil complex dielectric permittivity as well as the amount of water in soil. (Topp et al., 1980; Noborio, 2001)	– Commonly recognized alternative for the thermogravimetric method – Instruments are still very expensive – Usually no site calibration required
	Attenuation of the electromagnetic wave during its travel in the TDR probe, which results mainly from the soil electrical conductivity-dependent ion conduction. Signal attenuation is correlated with the soil bulk electrical conductivity and soil salinity defined as electrical conductivity of soil extract. (Malicki and Walczak, 1999; Robinson et al., 2003)	– Not applicable for very saline soils and long probe rods – Limited accuracy caused by the possible change of the TDR probe geometry
FDR (frequency domain reflectometry)	Phase shift (dependent on soil bulk dielectric permittivity) and amplitude attenuation (dependent on soil salinity) of a probe inserted into the soil treated as a lossy capacitor. Measurement is done in single frequency generated by the probe internal probe oscillator (50–150 MHz). (Veldkamp and O'Brien, 2000)	– Requires soil site calibration – Probes and meters are commercially available and cheaper than TDR instrumentation – Low power consumption as compared to TDR technique
Neutron scattering	Number of slow neutrons that are produced from the collision of fast neutrons with hydrogen molecules in soil, which is linearly related to the soil volumetric water content. Fast neutron generator and the counter are installed in the vertical access tube for the measurements in different layers of soil. (Evett and Steiner, 1995)	– Requires soil-site calibration – Precise but expensive – Additional cost with special licensing, operator training, handling, radiation materials waste disposal – Health hazard
Tensiometry	Suction force or pressure exerted on a pressure transducer in a water-filled tube connected with soil matrix by a porous cap. The measured physical quantity is a matrix potential of soil water, which is a basic element of the total potential of water in the soil. (Mullins, 2001; Sisson et al., 2002)	– Limited range of work (down to about −85 kPa) – Require frequent servicing (air bubbles) – In drought conditions water moves from the tensiometer to the soil
Electrical resistance blocks	Electrical resistance, measured with an alternating current bridge (usually ≈1,000 Hz) of electrodes encased in some type of porous material (gypsum, nylon fabric, fiberglass) that within about 2 days will reach a quasi-equilibrium state with the soil. This method determines soil water content and water potential as a function of electrical resistance. (Hillel, 1998; Spaans and Baker, 1992)	– Sensitive to soil salinity and temperature – Requires soil-specific calibration – Very economic and field installations can work for several years – Supplementary to tensiometers in the range up to −1,500 kPa
Nuclear magnetic resonance (NMR) spectroscopy	Structure and composition of soil, soil organic matter and nutrients (Randall et al., 1997), plant nitrogen metabolism. (Mesnard and Ratcliffe, 2005)	– High spectral resolution – Problems with equipment availability
X-ray computed tomography	Description and quantitative measurements of soil structure elements, especially of soil pores and pore network features, investigation the hydro-physical characteristics of the soil, in a functional and temporal manner, analysis of the biotic factor influence on soil. (Taina et al., 2008; Peth et al., 2008)	– High spatial resolution (∼ 1 μm) – Lack of unity, not only in the utilized methods, but also in terminology

There is a tendency to construct noninvasive integrated sensors that measure more than one physical soil property at the same time and in the same soil volume, for example, TDR or FDR soil water content and soil salinity integrated with an easy to implement temperature sensor (Skierucha et al., 2006), bulk density, and water content using low- and high-energy sources for CT scanning (Rogasik et al., 1999; Lipiec and Hatano, 2003), penetrometers with TDR probe sensors (Young et al., 2000; Vaz and Hopmans, 2001) and with thermal sensors (Marczewski et al., 2004), combined measurements system of TDR and tensiometry (Malicki et al., 1992; Walczak et al., 1993; Whalley, 1993), thermo-time domain reflectometry probe for measuring soil thermal properties and water content (Ren et al., 2003; Usowicz et al., 2006).

Summary

Nondestructive measurement methods in soil and other environmental objects develop rapidly following the technological advances in electronics, informatics, and materials engineering. They are on the application front of modern technology developments. Agrophysics should take advantage of the progress of nondestructive methods of measurements in medicine, satellite, and others branches of science financially supported by governmental and private funds and look for the new applications in the field of food quality and environmental protection.

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Cross-references

Electrical Properties of Agricultural Products
Electrical Properties of Soils

Magnetic Resonance Imaging in Soil Science
Nondestructive Measurements in Fruits
Noninvasive Quantification of 3D Pore Space Structures in Soils
Precision Agriculture: Proximal Soil Sensing
Remote Sensing of Soils and Plants Imagery
X-Ray Method to Evaluate Grain Quality

NONINVASIVE QUANTIFICATION OF 3D PORE SPACE STRUCTURES IN SOILS

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Definitions

Noninvasive research facilitates the understanding of physical, chemical, and biological processes in soils and their dependency on soil structure. The most commonly employed method or device used for noninvasive examinations of porous materials and their 3D architectures is X-ray Computed (Micro)Tomography (XCT, µCT), which can be either based on synchrotron radiation (SR-µCT) or microfocus tube sources (MF-µCT).

XCT = X-ray computed tomography
µCT = X-ray computed microtomography
SR = Synchrotron radiation
SR-µCT = Synchrotron radiation–based microtomography
Voxel = Three-dimensional equivalent to pixel
CCD = Charge-coupled device

Introduction

Soil pore spaces are of interest to soil researchers for various reasons where the traditional soil science disciplines usually take different perspectives. The soil physicist, for example, treats soil pore spaces mostly with respect to water, gas, and solid particle movements, while the soil biologist and soil chemist understands pore spaces predominantly as an environment for root growth and microbial activity and a pathway to access and retain nutrients or contaminants, respectively. Recent research on the soil-microbe system emphasizes that the interaction of physical, biological, and biogeochemical processes occurring within soil pore space structures deserves more appreciation (Young and Crawford, 2004). Soil scientists now begin to recognize that the physical heterogeneity of soil structures controls both abiotic and biotic functions within soil habitats with feedback loops between the two. In other words, soil structure and its dynamic functional properties regulate soil biodiversity (Crawford et al., 2005; Ettema and Wardle, 2002) while soil microbes in turn can alter soil structure and hence pore spaces (Six et al., 2004). Detailed insights into pore space realms are important not only from a soil microbial habitat perspective. Given that the interacting mechanisms operate across scales virtually all soil environmental processes (from transport to sorption and turnover) maintaining biogeochemical cycling in the pedosphere depend on pore space structures.

How to study soil pore space structures

Past research on soil structure and its associated pore space was strongly based on traditional techniques, which can be distinguished into direct (e.g., thin section analysis) and indirect (e.g., water retention function) methods. Despite profound conceptual understanding on soil structure formation and stability has been achieved the major drawback of this traditional approach is that the techniques are either destructive (e.g., preparation of thin sections) or that results refer to statistical values averaged over a bulk volume (e.g., pore size distribution) lacking detail on the spatial configuration of pores. Another problem is that soil structure is inherently three dimensional and that 2D analysis from thin sections bears some risk for inaccurate interpretations of structural morphologies. When we consider the soil pore space as a dynamic, three-dimensional, interconnected network of voids with a complex hierarchical organization we have to acknowledge that traditional methods are insufficient for deriving an adequate quantitative characterization of pore space morphologies. Noninvasive imaging techniques have made significant progress in the last decade (Nondestructive Measurements in Soil) promising to overcome some of the limitations involved in studying dynamic 3D soil pore spaces.

Applications of X-ray computed tomography in soil structure analysis

X-ray computed tomography (XCT) is the most widely used noninvasive imaging technique to study soil structure. The technique was introduced in the discipline of soil science by the pioneering work of Petrovic et al. (1982) investigating soil bulk density and later followed up by Crestana et al. (1986), who studied the spatial distribution and temporal dynamics of water in soil. Both used medical scanners achieving a voxel resolution in the submillimeter range. Later efforts were made to extend the noninvasive visualization of pore spaces beyond larger macropores (>50 µm) toward smaller pore sizes down to the mesopore range (<10 µm). However, because of the strong X-ray attenuation of the mineral soil components, resolution is generally limited by the distance the X-ray beam has to travel from the entry to the exit of the specimen and hence decreases with increasing sample size. As a rule of thumb, the resolution achieved is in the range of 1/1,000 of the sample thickness. A main limitation of conventional medical scanners for analyzing small samples at high resolution, however, is that because they are built for larger objects (human bodies) they do not reach the required precision in terms of angular rotation of the detector and sample positioning during image acquisition.

With synchrotron radiation sources becoming more accessible to the scientific community, the potential of this high energy radiation for X-ray microtomography of environmental samples was recognized. Pioneering work on synchrotron radiation–based X-ray microtomography (SR-μCT) was conducted by Flannery and colleagues about 20 years ago (Flannery et al., 1987). They introduced SR-μCT as a "new form of microscope" that produces three-dimensional images with a spatial resolution comparable to that of a light microscope (~1 μm). The use of SR-μCT for analyzing soil pore spaces at micrometer resolution was introduced by Spanne et al. (1994) but surprisingly only recently the technique was applied to study small-scale soil structure of natural undisturbed soils (Altman et al., 2005; Feeney et al., 2006; Nunan et al., 2006; Peth et al., 2008a; Peth et al., 2008b). Synchrotron radiation sources offer a variety of special techniques (fluorescence, absorption, diffraction, infrared) providing excellent perspectives for plant and soil research with a superior performance in terms of sensitivity, speed, and resolution (Lombi and Susini, 2009). Recent developments of high-resolution laboratory μCT systems, however, will make X-ray computed microtomography (μCT) a more readily available tool in soil structure analysis allowing for the visualization and quantification of soil pore architectures at a resolution down to a few microns with a quality that is very close to what is obtained from SR facilities (Brunke et al., 2008).

Principles of X-ray computed tomography

X-ray computed tomography is based on the differences in X-ray attenuation where an incident beam of intensity I_0 is absorbed by the internal components of the radiated object resulting in a transmitted beam with reduced intensity (I). This relationship is described by Lambert-Beer's law:

$$I = I_0 \exp(-\mu D) \tag{1}$$

where μ is the overall linear attenuation coefficient (L^{-1}) and D is the sample thickness (L^{-1}). The linear X-ray attenuation coefficient (μ) is a function of density and atomic number of the components as well as the X-ray energy used. For porous media consisting of different phases (solid, water, and air) Equation 1 must be extended accounting for the different phase specific attenuation coefficients to

$$I = I_0 \exp\left(-\left[(1-\theta_\mathrm{p})\mu_\mathrm{s}\rho_\mathrm{s}D + \theta_\mathrm{p}\mathrm{S_w}\mu_\mathrm{w}\rho_\mathrm{w}D\right]\right) \tag{2}$$

where ρ_s and ρ_w are the densities and μ_s and μ_w the linear attenuation coefficients of solid matter and water, respectively. S_w denotes the water saturation and θ_p the total porosity. Due to the low linear attenuation of air, the contribution of the gaseous phase to the overall attenuation is considered negligible and therefore omitted in Equation 2.

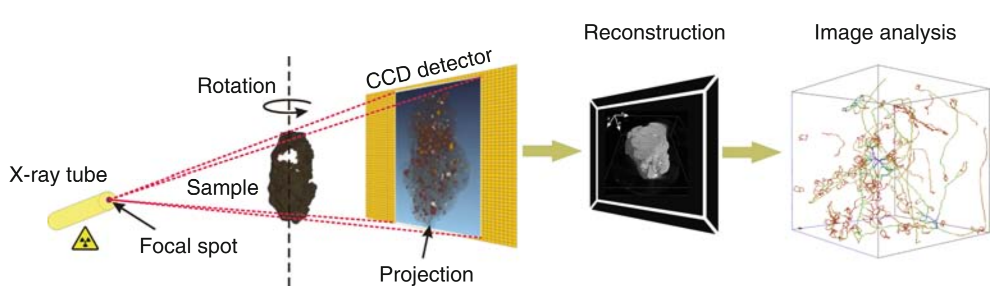
The incident fan-shaped X-ray beam is generated in a high vacuum X-ray tube and transmitted through the sample, which is mounted on a precision rotation table (Figure 1). The sample is rotated at 0.25–0.50° steps between 0° and 360° and at each angular step the integral attenuation of the X-ray beam transmitting the sample is recorded by the CCD detector. The measured angular projections of the sample are finally reconstructed into a 3D linear attenuation coefficient map. Commonly, attenuation coefficients are converted to grayscale values ranging from [255] for the highest attenuation coefficient to [0] for the lowest attenuation coefficient. Reconstructed images finally contain the spatial configuration of soil voids and soil components with sufficient attenuation contrast. Hence, the architecture of soil pore networks is available in digital format and can be analyzed quantitatively with 3D image analysis algorithms.

A readable introduction to principles of computerized tomography is given by Kak and Slaney (1988).

Visualization and quantification of soil pore space structures in 3D

During a microtomography scan usually a couple of hundred (often >1,000) grayscale image slices are recorded and subsequently rendered into a 3D volume of the sample. Tools exist to visualize the 3D structure of the sample providing some qualitative information about the pore space architecture, e.g., the spatial arrangement and continuity of pores. However, in order to make objective comparisons between different samples, some kind of morphological and topological quantification is desired.

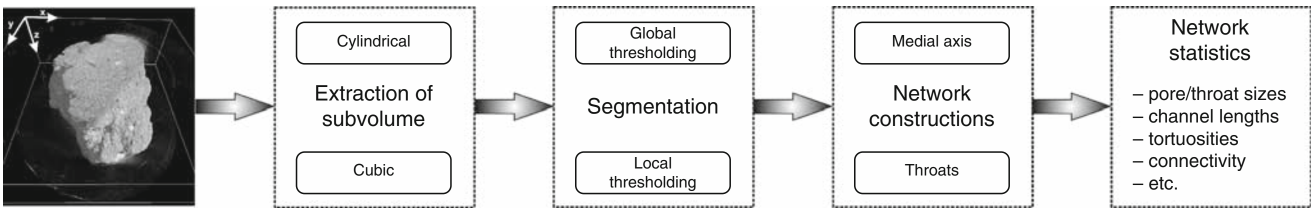
Morphological and topological features of pore networks may be quantified by means of 3D image analysis using algorithms that are based on the principles of mathematical morphology (e.g., Serra, 1982; Soille, 2003). Different sets of such morphometric algorithms that are suitable for analyzing soil pore spaces are available, e.g., *DXSoil* (Delerue and Perrier, 2002) and *3dma* (Lindquist



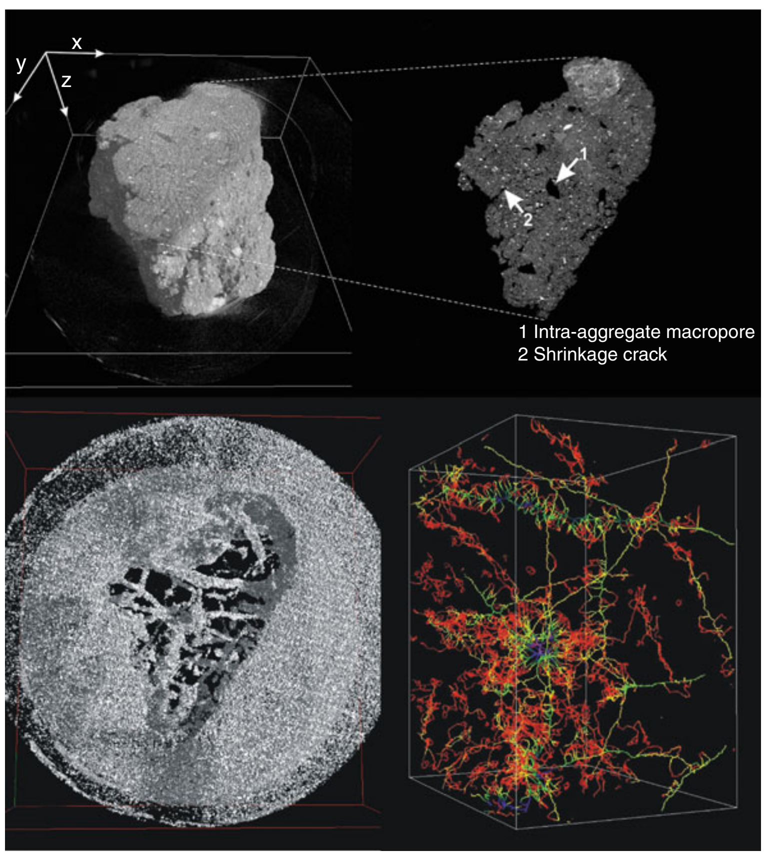
Noninvasive Quantification of 3D Pore Space Structures in Soils, Figure 1 Typical layout of a tomography experiment with a laboratory X-ray computed microtomography (μCT) system.

et al., 2005). Image analysis involves the stepwise transformation of the image data into sets (Horgan, 1998) from which a variety of geometrical features of the pore space structure can be calculated (e.g., size, shape, connectivity and tortuosity of pore channels; pore interface area; pore bottlenecks). Basic operations during image analysis with the software *3dma* are shown in Figure 2.

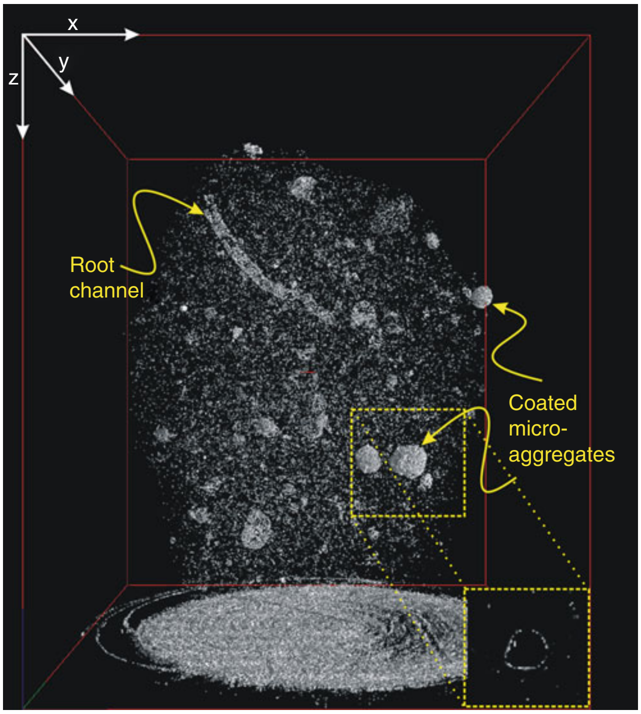
The application of *3dma* for analyzing the intra-aggregate pore space architecture of different soil aggregates was demonstrated by Peth et al. (2008a). Figure 3 shows an example of the reconstructed 3D X-ray attenuation map of a small-scale soil aggregate (5-mm diameter) and the extracted shape of the internal macropore architecture. The calculation of the skeleton (medial axis) reveals the existence of numerous convoluted narrow pores and a few continuous pore channels. Pore channels become visible when the 3D representation is restricted to a short range of grayscale values corresponding to specific attenuation coefficients. Obviously, larger pore channels are plagued with highly absorbing material in this case.



Noninvasive Quantification of 3D Pore Space Structures in Soils, Figure 2 Basic image analysis steps in *3dma*. (Reprinted from Peth et al., 2008b with permission from SPIE.)



Noninvasive Quantification of 3D Pore Space Structures in Soils, Figure 3 Three-dimensional reconstruction (*top*, *left*) of a soil aggregate (*Alfisol*, Rotthalmünster/Germany) and an *xy*-image slice showing shrinkage cracks and intra-aggregate macropores (*top*, *right*). Reconstructed pore channels (*bottom*, *left*) and medial axis representation of the main pore network (*bottom*, *right*). (Reprinted from Peth et al., 2008b with permission from SPIE.)



Noninvasive Quantification of 3D Pore Space Structures in Soils, Figure 4 X-ray attenuation map of a specific grayscale range of a paddy rice field soil aggregate (*Stagnic Cambisol*, Yingtan/China) showing coatings around root channels and microaggregates.

This phenomenon is also often visible around root channels and microaggregates (Figure 4).

Summary

Functional traits of soil structure, irrespective of scale, rely on the connectivity, tortuosity, and the heterogeneity of pore spaces in 3D (Young et al., 2001). This is often neglected using conventional approaches of investigating soil structure morphologies. Data concerning 3D architectures of pore spaces are invaluable when studying structural genesis, gas and water transport, habitat functions, water uptake, etc. Visualizing and quantifying the complex geometry of the pore network and soil structure on various scales is promising to enhance our understanding of the multiple interacting physical, biological, and biogeochemical processes taking place in soil pore spaces.

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Cross-references

Microbes and Soil Structure
Microbes, Habitat Space, and Transport in Soil
Nondestructive Measurements in Soil
Pore Morphology and Soil Functions
Soil Aggregates, Structure, and Stability
Soil Structure, Visual Assessment

NON-LIMITING WATER RANGE (NLWR)

See *Soil Physical Quality*

NON-THERMAL TECHNOLOGIES

See *Thermal Technologies in Food Processing*

NORMAL STRESS

See *Soil Compactibility and Compressibility*

NUMERICAL METHODS (MODEL)

Algorithms that use arithmetic and logical operations to obtain approximate solutions to complex formulas, such as differential equations, describing a soil process.

Cross-references

Agrophysics: Physics Applied to Agriculture