# PHYSICAL PROPERTIES OF SOLID AND FLUID MATRICES

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The unsaturated zone consists of a complex arrangement of solid, liquid, and gaseous phases, most of them interconnected. The spatial distribution and geometrical arrangement of each phase, and the partitioning of solutes between phases, are controlled by physical, chemical, and biological processes. Since the upper part of the vadose zone is the most dynamic region, and controls the further downward transport of mass and energy, the focus of this review is on the measurement, characterization, and interpretation of soil physical properties.

In essence, all soil physical properties, such as a soil's capacity to retain and conduct water and its dissolved solutes an other fluids, its thermal properties, and its strength, are determined by soil composition, pore sizes, and pore size distribution. Measurement and interpretation of these properties are challenging because of their dynamic nature and spatial variability.

We will show that most of the transport characteristics of the vadose zone are controlled by the phase distribution and connectivity of the pore space. Hence, transport may be determined in principle by a single soil-water dependent formation factor. Considering the state of the art in current understanding of soil physical processes and properties, it is expected that significant developments will soon occur in the characterization of these issues, both on a landscape scale and in terms of pore-size scale measurements. It is expected that groundwater research will move increasingly towards the integration of physical, chemical, and biological sciences.

#### **1. Introduction**

The unsaturated zone consists of a complex arrangement of mostly connected solid, liquid, and gaseous phases. The spatial distribution and geometrical arrangement of each phase, and the partitioning of solutes between phases, are controlled by physical, chemical, and biological processes. The unsaturated zone is bounded by the soil surface at its upper limit and merges with the groundwater in the capillary fringe at the lower end. The distinction between groundwater and the unsaturated zone is determined by the degree of water saturation of the subsurface. In the groundwater, it is generally assumed that the pore space within the solid matrix is saturated with the liquid phase (mostly water) and that the hydrostatic pressure in the water is greater than atmospheric pressure. In contrast, the pore space in the unsaturated zone is only partly filled with water in the liquid phase, while the remaining space is occupied by the gas phase. Water in the soil matrix is held by pressure and adsorptive forces. The distinction between groundwater and water in the vadose zone is usually made within a hydrologic context, emphasizing water as the subsurface agent of change and the main driver in the transport of chemicals between the atmosphere and groundwater. Although the importance of water is paramount, it is becoming increasingly clear that chemical and biological components can also have a profound influence on the subsurface. It is for this reason that vadose zone notation is preferred, emphasizing the multidisciplinary approach needed for subsurface characterization.

The upper part of the vadose zone is the most dynamic, and changes occur within increasingly smaller time and spatial scales when moving from the groundwater towards the soil surface. The uppermost part of the vadose zone is subject to fluctuations in water and chemical content by infiltration and leaching, water uptake by plant roots (transpiration), and evaporation from the soil surface. Water is the main element leading to soil formation from the weathering of parent material such as rock or transported deposits; additional factors such as climate, vegetation, topography, and parent material also determine soil physical properties. Generally, the soil depth is controlled by the maximum rooting depth (usually confined within a few meters from the soil surface). However, the vadose zone can extend much deeper than the surficial soil layer and includes unsaturated rock formations and alluvial materials to depths of 100 m or more, determined by hydrologic, topographic, and lithographic characteristics. Most available vadose zone characterization techniques have been developed from soil physical measurements, prompted by research needs in agricultural sciences.

Unquestionably, human activities have had a negative impact upon the quantity and quality of natural soil, water, and air resources. Chemical pollution generated by agricultural, industrial, and municipal activities has contaminated soil, groundwater, and surface water systems worldwide. Scientists are now increasingly aware that soil is a

critically important component of the biosphere, not only because of its role in food production but also as the safeguard of local, regional, and global environmental quality. For example, it is believed that management strategies in the unsaturated soil zone will offer the best opportunities for preventing or limiting pollution, or for remediating ongoing pollution problems. Because chemical residence times in groundwater aquifers can range from years to thousands of years, pollution there is often essentially irreversible. Prevention or remediation of soil and groundwater contamination starts, therefore, with proper management of the unsaturated zone.

In the last few decades interest in the deeper vadose zones has increased, instigated by the need to sustain the quality of groundwater as a source of drinking water and for ecological purposes. Specifically, the evaluation of deep consolidated rock bodies' suitability for use as radioactive waste repositories has significantly increased research into the physical properties of fractured rock. However, we will focus here on the physical properties of unconsolidated porous matrices based on our experiences in the physical characterization of soils.

We will first consider the soil's solid phase and emphasize its importance in chemical and biological processes. For example, rates of chemical contaminant transport and maintenance of soil structure are largely controlled by soil composition. Recognizing the importance of water, we examine various soil–water interaction mechanisms and relate them to the main physical characteristics that control water flow. We will review some of the basic soil-mechanical, solute, and thermal transport properties, and conclude with a section on opportunities and challenges, laying out a roadmap of immediate needs in the area of physical characterization.

#### 2. Solid Phase

#### 2.1. Soil Composition

The porous matrix of the soil is the result of mechanical, chemical, and biological weathering of the original rock, or of transported parent material. As the upper part of the vadose zone, it serves as the major source of nutrients and water for crop and plant growth, and forms the main conduit between the Earth's surface and the groundwater. Hence, the principal soil physical properties heavily influence plant growth and water transport.

The soil consists of the solid, liquid, and gas phases. The *solid phase* is composed of mineral and/or organic matter, consisting of particles of (mostly) irregular shape, a large range in size, and varying chemical composition. The *liquid phase* is usually an aqueous solution, with physical and chemical properties varying in both space and time, depending on the degree of solid–liquid interaction as determined by solid material composition and environmental variables such as temperature and the chemical composition of the original water. However, in some specific situations the liquid phase may be a *nonaqueous phase liquid* (NAPL) with completely different fluid properties. Most NAPLs, such as oils and solvents, are immiscible with the water solution. The *gas phase* is usually composed of gases with concentrations approximately equal to those in

atmospheric air. Their concentration may vary, however, depending on plant and soil microbial activity, and on chemical reactions with the solid and liquid phases.

The exact geometry of the solid matrix and associated pore space is extremely complex, and generally impossible to describe in relation to its properties and function. Consequently, when characterizing soils we usually do so in terms of *effective* properties. For example, soil particle size distribution is based on equivalent particle diameters, and soil pores may be described with reference to capillary tubes with equivalent diameters. The solid phase is characterized by soil texture, chemical and mineralogical properties, shape and surface area, and soil structure. These properties combined will affect soil–water interactions, and transport and mechanical properties.

The individual particles that makeup the soil matrix vary in size with equivalent diameter,  $d_e$ , ranging from smaller than 0.1 µm (colloidal particles) or 2 micrometers (clay) to larger than 2 mm (gravel) or 75 mm (stones). Intermediate size fractions include silt with 2 µm <  $d_e$  < 50 µm and sand with 50 µm <  $d_e$  < 2 mm. Particle size distribution is determined by mechanical sieving for sizes larger than the silt fraction, and by sedimentation methods such as the pipette and hydrometer technique for the smaller sized fractions. A texture diagram, such as the US soil textural triangle, serves as a reference for soil classification.



Figure 1. Soil textural triangle

The mineral composition of the solid particles is determined by the parent material and the degree of weathering. The primary minerals are those that are present in the original rock, and are the most resistant to weathering. These include quartz, feldspars, and micas. The secondary minerals are formed by decomposition of the primary minerals, and their subsequent weathering and recomposition into new ones. These include soluble (gypsum, calcite) and nonsoluble (iron and aluminum oxides and hydroxides) minerals. The latter are often platelet- or lath-shaped, and are referred to as clay minerals. The type and relative amount of clay minerals present has an enormous influence on a soil's physical and chemical properties, determined by their crystal structure, surface area, and exchangeable cations. Clay minerals consist of stacks of unit layers or building blocks of crystal lattices (thickness of 0.5–1.0 nm) that are formed by sharing oxygen atoms between tetrahedral (four oxygen atoms are coordinated around one silicon atom) and octohedral (six oxygen atoms or hydroxyls are coordinated around one aluminum or magnesium atom) sheets. In kaolinite minerals, the building blocks consist of one tetrahedral and one octahedral sheet (1:1 mineral), which are held together by hydrogen bonding. In contrast, the building blocks for micas (illites and vermiculites) are composed of two tetrahedral sheets combined with one octahedral sheet (2:1 minerals), mainly bonded by non-exchangeable potassium ions. In contrast once more, the 2:1 unit layers of smectite clays are bonded by exchangeable cations. The type of bonding between the unit layers controls cation exchange capacity, effective surface area, and soil swelling.

Clay minerals are characterized by a net negative charge, caused by isomorphous substitution between atoms of equal size but with a lower positive charge (e.g.  $Al^{3+}$  for Si<sup>4+</sup>) during the soil weathering process. Consequently, cations are concentrated at the clay surfaces to compensate for this net negative charge, of which the type of exchange is governed by the Coulomb attraction forces. For example, higher-valence cations are usually more attracted to the negative surfaces than lower-valence ions. The thickness of the water film around the mineral surface where the cation concentration is larger than in the bulk solution is defined as the diffuse double layer (DDL). The pHdependent capacity of exchangeable cations is described by the cation exchange *capacity* (CEC, meq kg<sup>-1</sup>). This is lowest for kaolinite (about 100), whereas it is about 300 for illite and 1500 meq kg<sup>-1</sup> or more for montmorillonite. The CEC values of the different clay minerals increase with their respective surface areas: viz.  $5-100 \text{ m}^2 \text{ g}^{-1}$  for kaolinite, 100–500 m<sup>2</sup> g<sup>-1</sup> for micas, and 700–1000 m<sup>2</sup> g<sup>-1</sup> for smectites. Oxides and organic matter also contribute to the bulk soil CEC. Upon wetting of clay, the water molecules are attracted to the exchangeable cations by osmosis, thereby causing a first stage of swelling. Depending on the clay mineral type, soil solution concentration, and dominant valence of the exchangeable cations, continued hydration may occur causing further soil expansion, swelling pressures, and ultimately soil dispersion. Soil swelling can cause soils to become impermeable and prevent gaseous exchange between the soil and atmosphere. Subsequent drying causes soil subsidence. Both processes may cause damage to buildings, pavements, and pipelines. Soil shrinkage and cracking result in preferential, downward flow of water and dissolved chemicals beyond the rooting zone. The relative abundance of the different clay minerals can be determined from x-ray diffraction analysis.

Many physical and chemical properties of soil are determined by processes at solidliquid interfaces. Examples are chemical adsorption, swelling potential, soil water retention and conductivity, and soil structural properties. Hence, the *soil specific surface area* ( $S_m$ , m<sup>2</sup> kg<sup>-1</sup> dry soil) is an important physical property of soil in addition to soil texture and mineralogy. Because of variations in soil composition and mineralogy, the surface area of the bulk soil is a mass-weighted mean specific surface area of the various components. It can be directly measured from the known particle distribution and geometry, or from heat of wetting and liquid adsorption techniques when the exact particle geometry is unknown. To illustrate the effect of size on soil-specific surface area, the geometrical method will be demonstrated by assuming that the soil particle shape is known. For example, if the solid particles are assumed to be spherical (with radius *r* and particle density,  $\rho_s$ ) the specific surface area is computed from the ratio of solid particle area ( $a_s$ ) and mass ( $m_s$ )

$$S_{m} = \frac{a_{s}}{m_{s}} = \frac{4\pi r^{2}}{\rho_{s}(4\pi r^{3}/3)} = \frac{3}{\rho_{s}r}$$

For disc-shaped clay particles with thickness *t* and disc radius r >> t, a similar expression yields a specific surface area of  $2/t\rho_s$ . It is evident that  $s_m$  is inversely proportional to particle size, resulting in a proportional increase in bulk soil specific surface area with a decrease in average particle size across a range of particle shapes. For example, a sand particle with an effective diameter of 0.2 mm has a specific area of  $11.3 \text{ m}^2 \text{ kg}^{-1}$ , while disk-shaped clay particles with 1 nm thickness have a specific area of  $750 \times 10^3 \text{ m}^2 \text{ kg}^{-1}$  or  $750 \text{ m}^2 \text{ g}^{-1}$  soil, assuming  $\rho_s = 2650 \text{ kg m}^{-3}$ .

(1)



Figure 2. (a) Two vertical cross-sections of a glass-bead pack with REV of 140 voxels (2.576 mm) side length. Pore space is occupied by air. Gray scale maps attenuation values between  $-0.01 \text{ mm}^{-1}$  (black) and  $0.07 \text{ mm}^{-1}$  (white). Bead diameter is 0.5 mm. (b) Estimated porosity for a cubic domain of increasing size within a glass-bead pack, centered within either the air or the glass phase. Cube side length is expressed as multiple of the bead diameter  $d_p$  (0.5 mm).

When determining the bulk soil surface area or any other soil physical property, the required sample size should be considered critically. Since it is fair to state that available measurement techniques and associated conceptualizations are unable to describe the exact microscopic geometry, porous medium properties and processes are treated at the macroscopic level, with continuous property values across the spatial domain. In this approach, one takes a point within the porous medium volume and considers the representative elementary volume (REV) around it. The REV size must be such that a meaningful average value for a given property is obtained. The REV concept is demonstrated in Figure 2 for the porosity of a medium composed of glass beads. Beads of uniform size are packed randomly into a vertical Plexiglas cylinder of 4.76 mm inner diameter (Figure 2a). The porosity is determined as a function of volume size using x-ray CT. This technique allows the average density to be measured at a spatial resolution of about 20  $\mu$ m. The bead diameter  $d_p$  was 0.5 mm. By selecting the point in either a glass bead or a pore, measurement volumes were increased by integrating voxel attenuation values within the selected volumes of cube side L. As expected, porosity values are quite different at the smaller measurement volumes, but both curves meet (Figure 2b) and remain constant once a REV size,  $L/d_p$ , of about five times the beads' diameter has been reached.

#### 2.2. Soil Structure

The arrangement of individual soil particles, and their tendency to bind together in aggregates of different sizes, shapes, and arrangements, is defined as soil structure. The cementing agents can be of biological, physical, and chemical origin. Aggregation creates intra-aggregate and inter-aggregate pore spaces, thereby significantly altering flow paths through the soil for water, gases, and solutes. Soil structure generally leads to an increase in total pore space, a corresponding decrease in soil bulk density, and an increase in the size distribution of soil pores. Lack of soil structure affects plant growth adversely through reduction in aeration, higher levels of soil compaction, and limited root exploration. The presence of soil structure is, however, generally considered unfavorable in the context of engineering applications. In various ways, soil structure— or the lack thereof—can have a major influence on contaminant transport. Soil structural development is influenced by:

- the amount and type of clay minerals, as well as the type of exchangeable ions present;
- the amount and type of organic matter; and
- the presence of iron and aluminum oxides and hydroxides, and of other inorganic precipitates such as lime and gypsum.

In the presence of clay, water can effectively act as a bridge, connecting soil particles through cation–water dipole interactions, whereas organic matter provides a nutrient source for soil fungi and bacteria that produce the cementing agents through the secretion of polysaccharides. Humus, which is a stable form of organic matter, acts like a clay mineral, with a CEC and adsorbing cations. Structure is enhanced by various mechanisms that bind organic and inorganic compounds, and by plants through their production of organic material (OM), their protection of the soil surface, and the role of their fibrous roots in holding the soil together.

Soil structure is a dynamic property which deteriorates with soil wetting, tillage and cultivation, and a decrease in OM. Soil wetting will generally reduce the binding forces between soil particles, but its effect depends on electrolyte type and concentration. For example, sodium ions in the soil solution increase the exchangeable sodium percentage (ESP). Their presence tends to increase the osmotic pressure and the extent of the diffuse double layer (DDL) upon wetting, thereby causing swelling and possibly dispersion of soil, and the associated collapse of the soil's hydraulic conductivity (sodic soils). Specifically, rainfall causes aggregate breakdown due to the energy impact of the falling raindrops. This causes soil slaking and the formation of relatively impermeable surface layers or crusts, which in turn lead to accelerated surface water runoff and soil erosion. When soil stresses, like those caused by tillage and cultivation, are larger than the cementing forces, aggregate breakdown and soil compaction results. A soil's structural stability is closely related to the continuous supply of organic matter to it. Because of its dynamic nature and its instability, soil structure makes it difficult to quantify. Hence, characterization of soil structure is mostly done using qualitative methods such as morphological classification. Quantitative measurement involves determining particle-size distribution using dry and wet sieving techniques, porosity and pore-size distribution employing mercury intrusion or water desorption methods, hydraulic conductivity and water infiltration measurements, and soil compaction methods involving bulk density or soil strength measurements.

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#### **Biographical Sketches**

**Dr. Jan W. Hopmans** is full professor in the Hydrology Program of the Department of Land, Air, and Water Resources at the University of California, Davis. He graduated from Wageningen Agricultural University, the Netherlands, with an M.Sc. degree in hydrology, and in 1985 obtained a Ph.D. degree in soil physics from Auburn University. Since joining the faculty at UC Davis in 1988, he has published over 100 scientific research papers in peer-reviewed journals, and he has co-edited two books. His research and teaching is focused on vadose zone hydrology and soil physics, and includes interests in unsaturated flow and transport, contaminant hydrology, x-ray microtomography, root–soil water interactions, parameter optimization, and irrigation water management. He teaches undergraduate and graduate courses in soil physics, irrigation water management, and vadose zone modeling, and was Director of the Hydrology Program for almost three years. He has been Associate Editor of the *Soil Science Society of America Journal*, and is a currently member of the Editorial Board of *Advances in Water Resources, Soil Science Reviews, Vadose Zone Journal, and International Agrophysics*. He was Chair of Division S-1 (Soil Physics) of the Soil Science Society of America (SSSA) in 1999–2000, and was elected Fellow of the SSSA in 1999. He was awarded a LWRRDC fellowship to allow him to undertake a one-year sabbatical with CSIRO Land and Water in Townsville (Queensland), Australia.

Dr. Jacob H. Dane is an alumni Professor of Soil Physics in the Agronomy and Soils Department at Auburn University. He has a B.Sc. degree in agricultural engineering from Wageningen Agricultural University, the Netherlands, an M.Sc. degree in soil physics, with a minor in civil engineering, from New Mexico State University, and a Ph.D. degree in soil physics, with a minor in mathematics, from Colorado State University. Dr. Dane's research interest is in flow and transport through porous media. He is specifically interested in three topics: the determination of soil hydraulic properties by direct and indirect methods; density-effected flow and transport of miscible fluids; and multi-fluid flow, including that of dense non-aqueous liquids. He has published 66 refereed journal articles and over a hundred symposia, abstracts, and miscellaneous publications. He has taught experimental and theoretical soil physics for 24 years. Dr. Dane was a Senior Research Fellow at the Wageningen Agricultural University, the Netherlands, a Research Fellow at Colorado State University, and a visiting professor at the University of Agricultural Sciences Vienna. He was awarded the Senior Research Award of the Alabama Agricultural Experiment Station, and is a Fellow of the Soil Science Society of America (SSSA) and of the American Society of Agronomy. He has been an Associate and a Technical Editor of the SSSA Journal and has served on several SSSA committees. He is currently Co-Editor of Methods of Soil Analysis, Part 1, Physical Properties, for the SSSA.