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TRANSPORT PROCESSES IN SOILS AND ITS HETEROGENEOUS BEHAVIOUR

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1. INTRODUCTION

Investigation of the effect of soil structure on relevant physical processes such as mass transport and biochemical transformations is an area of intense research interest. Soils, as many other porous media are generally not homogeneous. The underlying heterogeneity of the medium may induce particular physical phenomena that standard theories developed for homogeneous porous media are inadequate to describe.

In what follows we shall distinguish structural and functional variables of a porous medium. Structural variables refer to morphological and topological properties and functional variables describe physical processes occurring in the medium. The purpose of this contribution is to analyze the relationship between structural and functional heterogeneity in soils.

But what do we mean by heterogeneous? At a given scale, a physical property is homogeneous if it is invariant under translations and rotations of the space-time domain. As the description of any physical property or process depends on the scale of observation, heterogeneity is scale dependent. At the *microscopic or pore scale*, a porous medium may be viewed as a distribution of solid in the continuous space. Structural homogeneity implies the same probability of finding a solid particle everywhere (solid particles randomly or regularly distributed).

Usually, a process of scaling-up from the microscopic scale is used to adequately deal with measurable and observable quantities in porous media. Scaling-up involves averaging and smoothing out the complexity of the system. A point of the scaled-up space-time domain represents a volume of the smaller scale space-time domain. The up-scaled space is constructed by mapping each volume into a point. Each point of this macro-space contains implicitly the information of the microscopic solid distribution within the averaging volume. A macroscopic point to point structural variable, the porosity, may be defined to characterize the up-scaled porous medium. In order to define the up-scaled space as a continuum the porosity should vary smoothly in space, it should not diverge at any point in the mathematical sense (Baveye and Sposito, 1984; Bear and Bachmat, 1990). The averaging volume must then be “nearly” homogeneous with respect to the microscopic solid distribution in the sense above defined. This “nearly” invariant averaging volume is usually called the representative elementary volume. If the volume is strictly invariant the up-scaled medium is continuous and structurally homogeneous. Bear and Braester (1972) stated that the invariance property implies that the structural variables must be stationary under first order changes in the averaging volume. This is equivalent to requiring a slow and smooth variation of the averaged variables in space.

Let l , L and L^* be, respectively, the typical lengths of the pore, up-scaled continuous and up-scaled homogeneous spaces. Then $l \ll L < L^*$. At observation scales of typical length $l^* < L$ the medium

will be discrete and show high structural heterogeneity. For $L < L^*$ the medium is continuous and heterogeneous in the sense that structural variables show smoothly varying spatial variability.

At any scale, functional processes are completely defined by a set of conservation laws for the relevant physical variables. These equations are called *the constitutive equations* of the system at the corresponding scale. The system evolves in a space-time domain, and the physical variables are point to point functions of the space and time coordinates. The up-scaling process may be applied to any physical variable. The set of scaled-up physical variables is obtained by averaging the corresponding small-scale variables over a nearly invariant volume. If the averaging volume is the same for all the functional and structural variables involved in a given process, the up-scaled constitutive relations may be obtained. The constitutive equations involve a number of coefficients, which are scalar, vector or tensor quantities called *the transport coefficients*. These coefficients depend on the underlying structure of the space-time domain (e.g., symmetries, heterogeneity), and of the physical laws at scales below the observation scale (Wolfram, 1986). At any scale of description, the complexity of the system observed at more detailed scales is smoothed out, but microscopic information appears in the transport coefficients as well as in the form of the constitutive equations.

Detailed scales such as the pore scale imply many degrees of freedom to handle. Though theoretically we can always construct a continuous up-scaled space where we can define smooth varying transport coefficients and variables, in many cases it is impractical because this scale may not correspond to our observation or measurement window range scale.

For practical applications in Soil Science we are interested in describing transport and other physical phenomena in spatial domains having a typical length of at least a few centimeters which corresponds to our observation natural range scale. This is what is usually called the *macroscopic scale*. In general, the typical length of our macroscopic observation scale is smaller than L^* and it is often smaller than L . Thus soils at our measurement scale present various degrees of heterogeneous structural patterns from smoothly varying to discrete divergences. As a consequence, physical processes such as mass transport are also heterogeneous.

An external source of heterogeneity, non-intrinsic to the medium, is originated by the presence of biological agents within the soil (microorganisms, roots and microfauna). Besides, soil structure evolves in time inducing time heterogeneous processes.

In what follows we shall focus on multiple-scale structural and functional heterogeneity.

2. STRUCTURAL AND FUNCTIONAL HIERARCHY IN SOILS

Most soils at the macroscopic scale show functional and structural hierarchy. These concepts have been introduced by Cushman (1990). A porous medium has structural hierarchy if it can be

decomposed into successively nested, interacting physical sub-units. Functional relates to hierarchical processes within the porous medium. As mentioned above these two types of hierarchy are intimately connected.

The hierarchy is discrete if there are a finite number of nested structural sub-units or functional sub-processes and it is continuous otherwise. For a continuous hierarchy the number of subunits or processes goes to infinity and no clear-cut decomposition is in evidence.

Let us classify, as Cushman, natural soils at the macroscopic scale into three main groups:

a. Soils with one length scale

Let l^* and L be, respectively, the typical length of our macroscopic scale of observation and the minimum length scale for the continuum approach to be valid. When l^* is of the order or greater than L the observed soil will have only one macroscopic length scale. For these soils, the dispersion of the porosity is small, and its variation may be represented by a continuous function of the spatial coordinates.

b. Soils with two separated length scales

In this case the medium is continuous but for a number of discrete divergences of the porosity. In this type of soils, cracks, or fractures are distributed within a continuous matrix. The macropores have a mean aperture, that is several orders of magnitude greater than the mean length characterizing the pore size of the matrix. There are hardly any soils having two well-separated scales, however, this idealization may apply in certain cases like tropical vertisols.

c. Soils with continuous or successively nested length scales

In the general case, soil porosity shows a nearly continuous distribution of void sizes, ranging from micrometers to centimeters. The frequency distributions of void size classes are not homogeneous, the larger sizes usually represent only a small portion of the total porosity. Packing voids, pore necks, vughs, irregular channels of different sizes are usually present in soils. The continuous approach is not valid at the macroscopic observation scale.

We shall hereafter analyze the applicability of macroscopic transport equations for each group of soils.

3. MASS TRANSPORT AS AFFECTED BY SOIL STRUCTURAL HIERARCHY

3.1 Macroscopic mass transport equations for soils with one length scale

The macroscopic mass transport equations for soils with one length scale are well established. Under the assumption of continuity, these equations have been derived from the microscopic basic conservation principles for mass and linear momentum at the pore scale by using different techniques:

simple volume averaging (Bachmat and Bear, 1986; Bear and Bachmat, 1986; Whitaker, 1986), convolutions with weighting functions (Baveye and Sposito, 1984) or more general filters (Cushman, 1984). The macroscopic equations have also been obtained by the multiple-scales or perturbation method (Saez et al., 1989).

In what follows we shall focus on water transport. The macroscopic conservation laws for linear momentum and mass are derived from the corresponding microscopic equations (Bear and Bachmat, 1990).

The *macroscopic momentum balance equation* for the water phase is:

$$\underbrace{\theta \left[\frac{\partial (\mathbf{u}/\theta)}{\partial t} + \frac{\mathbf{u}}{\varepsilon} \cdot \nabla (\mathbf{u}/\theta) \right]}_{[a]} = \underbrace{-\frac{\theta}{\rho} \mathbf{A} \cdot [\nabla p + \rho \nabla(gz)]}_{[b]} + \underbrace{\nu \nabla^2 \mathbf{u}}_{[c]} - \underbrace{\nu \mathbf{B} \cdot \mathbf{u}}_{[d]} \quad [1]$$

In the above equation, $\mathbf{u} = \theta \mathbf{v}$ is the volumetric water flux. θ and \mathbf{v} are, respectively, the volumetric water content and the macroscopic water velocity. ρ , p , g , ν and z are, respectively, the macroscopic fluid density, pressure, acceleration due to gravity, kinematic viscosity and the spatial coordinate parallel to the gravity force. \mathbf{A} and \mathbf{B} are second order tensors related, respectively, to the microscopic tortuosity of the void space, and to the microscopic solid-void distribution.

Equation 1 is the macroscopic analog of the Navier-Stokes microscopic equations (Landau and Lifchitz, 1971), except for the damping term [d]. The term [a] represents the total inertial force per unit volume of porous medium, part [b] is the total force exerted on the fluid by pressure and gravity, and term [c] is the viscous resistance exerted within layers of the fluid due to internal friction. This term is of diffusive type, and shows that the velocity field will diffuse with a coefficient of diffusion ν . [d] represents the viscous resistance to flow due to the presence of the microscopic solid boundaries. From a macroscopic point of view, the solid distribution exerts a force on the fluid in the porous continuum proportional to its velocity, and all the information on the microscopic distribution is contained in the coefficient \mathbf{B} .

The *mass balance equation*, written for the water phase, leads to the macroscopic continuity equation:

$$\frac{\partial \theta}{\partial t} + \nabla \cdot \mathbf{u} = 0 \quad [2]$$

Equations 1 and *2*, with the boundary conditions for each particular problem, completely define the flow system.

Darcy's empirical law may be derived from *Equation 1*, under the restriction that the resistance to flow due to the presence of the solid is dominant with respect to inertial effects and to momentum diffusion

due to viscosity within the fluid. Then, the terms [a] and [c] in *Equation 1* may be dropped which leads to the well-known relation:

$$\mathbf{u} = -\mathbf{K} \cdot \nabla H \quad [3]$$

where

$$H = \frac{p}{\rho g} + z, \quad [4]$$

is total water potential, and

$$\mathbf{K} = \frac{\mathbf{A} \cdot \mathbf{B}^{-1} \theta \rho g}{v} \quad [5]$$

is the hydraulic conductivity tensor. This tensor captures all the microscopic effects due to the presence of fluid-solid boundaries. The combination of *Equation 3* with *Equation 2* yields Richards' transport equation (Richards, 1931).

$$\frac{\partial \theta}{\partial t} + \frac{\partial K}{\partial \theta} \nabla \theta = \nabla \cdot (D \nabla \theta) \quad [6]$$

where $D = K \frac{\partial H}{\partial \theta}$ is the diffusivity

No functional differentiation of the various void sizes is observed at the macroscopic scale, and the underlying information on the microscopic structure is contained in the transport coefficients K and D . These coefficients imply momentum dissipation towards the solid at the REV scale (Germann and Di Pietro, 1999). For a macroscopic observer, the flow is smooth and continuous, and the hydrodynamic processes approach the thermodynamic equilibrium. Flow can be treated as reversible diffusion of the total water potential.

3.2 Heterogeneous Mass Transport Processes in Soils

One of the most challenging research subjects in Soil Science is the description of heterogeneous water transport. This process is called preferential, macropore, or by-pass flow and refers to a fast infiltrating response to rain along certain soil pathways. Under certain boundary and initial conditions, preferential flow governs the soil-water regime. To some extent, by-pass flow occurs in most soils where roots, earthworm channels, cracks, and fissures of varying sizes are nearly always present. Structured clay soils, plow layers of agronomic soils, and forest soils with low bulk densities are just a few examples. In them rapid drainage and irregular flow patterns are widespread, and Darcy's regular, smooth flow is an idealized simplification. Preferential flow does not always occur, because input

intensities, vertical continuity of meso and macropores, and initial soil water may combine to determine its occurrence (Di Pietro, 1990; Di Pietro, 1993; Di Pietro, 1996; Germann and Di Pietro, 1996).

The geometric arrangement of voids determines the degree of heterogeneity of the water front. Driving and resistance forces determine the mean water velocity in each void. As a consequence, the average velocity of the flow varies with regard to the geometry and the size of the voids. Water advances rapidly in the wider pores because they exert less resistance. For these soils, multiple space-time scales appear necessary in the description of transport.

3.2.1 Water Transport in Soils with two separated length scales

The hydrodynamic response of the two distinct length scales is quite different. Within the cracks, preferential flow may occur. The time scale of this process is very different from that of the flow in the matrix. While the infiltration and redistribution of water within the matrix is a slow process of the order of days to months, the rapid drainage response to rain may last from minutes to hours (Germann, 1986). In this case, the continuum hypothesis does not apply to the entire medium, because macroscopic discontinuities are present.

Many authors (Barenblatt et al., 1960, Hosang, 1993; Jarvis, 1994) approached transport in these double porosity media, by conceptualizing them as superposition of two interacting continua, one representing the macroporosity and the other the microporous matrix. Usually, two macroscopic continuity equations, one for each continuum, are used to describe the system, coupled by a source-sink term accounting for the volume exchange of fluid between the two continua. These equations are:

$$\frac{\partial \theta_{1,2}}{\partial t} = -\nabla \cdot \mathbf{u}_{1,2} \pm S \quad [7]$$

where the index 1 and 2 indicate the matrix and the fractures, respectively, and S is the source-sink term. To solve this coupled system, we need to relate \mathbf{u} and S with measurable macroscopic physical variables in each continuum. Within the matrix, it is supposed that *Equation 3* is valid, and thus for the matrix flux it holds

$$\mathbf{u}_1 = \mathbf{K}_1 \cdot \nabla H_1 \quad [8]$$

Let us analyze *Equation 1* for flow within fractures. The damping term [d] may be neglected, as we may suppose that the resistance force due to solid walls is very small. Even if there is not convincing experimental evidence, the inertial term is also supposed to be small with respect to the diffusive viscous term. This assumption is equivalent to admitting quasi-steady flow conditions and that the Reynolds number of the flow within the fractures is small. Under these assumptions, *Equation 1*, written for the fractures, results in

$$\nabla^2 \mathbf{u}_2 = \mathbf{R} \cdot \nabla H_2 \quad [9]$$

where $\mathbf{R} = \theta g \mathbf{A} / \nu$ is a second order tensor, depending on the microscopic configuration of the fluid and of the tortuosity of the macropore void space within the REV.

If we assume that the total potential only depends on the vertical coordinate (z-axis) and that the fractures are vertical tubes of simple geometry, *Equation 9* reduces to

$$\frac{\partial^2 u_{2z}}{\partial y^2} + \frac{\partial^2 u_{2z}}{\partial z^2} = R_{zz} \frac{\partial H_2}{\partial z} \quad [10]$$

which may be solved with the boundary conditions $u_{2z} = 0$ on the walls of the tubes.

If the tubes are cylindrical or planar, the solution of *Equation 10* leads to Poiseuille's law for the volume flux in fractures. But, even in this simple case, the flux depends on the unknown coefficient R_{zz} . Many dual models suppose that the macropore system consists of interconnected tubes of simple geometry, possibly with varying apertures. Poiseuille's law is supposed to be valid for the fractured system. Empirical or numerically calculated coefficients are introduced to account for the variability of the fracture apertures (Moreno et al., 1990; Wang and Narasimhan, 1985).

The fluid exchange between the two continua is generally supposed to be proportional to the potential difference between the two media. The potential is assumed to be well-defined everywhere in each continuum, and that quasi-steady conditions hold for the inter-continuum flow. Two fluxes and two potentials are assigned to each point of the space in this approach, leaving the double continuum approach ill-defined from the physical point of view. However, it may produce solutions of practical interest like the case of fractured rock reservoirs in the saturated zone, where the assumptions about the fluxes in the fractures seem not to be far from reality.

Durner (1994), among others, introduced bi-modal shaped potential functions allowing to extent the hydraulic conductivity function for dual-porosity media. The underlying assumption is the validity of Darcy's law in the macropore domain. Although this assumption is inaccurate at the macroscopic scale, the use of a bi-modal coefficient ameliorates the description of flow near saturation.

In general, it is difficult to accept, for instance, the quasi-steady conditions for flow in the wider cracks. The cracks may carry water very deep in a short time after heavy rains. In that case, the inertial term of *Equation 1* cannot be neglected. Furthermore, how can the instantaneous value of the potential in the macropore continuum be defined under these rapid transient conditions?

Alternatively, if it is considered that the flux within the fractures is a single-valued function of the fluid volumetric fraction, *Equation 7*, may be transformed into a kinematic wave equation (Lighthill et al., 1955; Majda, 1984), which may be solved by the method of characteristics (Abbot, 1966). By assuming that the relation

$$u_2 = b\theta_2^a \quad [11]$$

holds for the fractures, Germann (1985) obtained traveling wave solutions for the flux within the macropores for a square pulse input.

It has been shown (Di Pietro and Lafolie, 1991) that this approach applies reasonably well to water content profiles for high water input rates and high degrees of saturation. Yet the meaning of the parameters involved in the equation and the limits of application of this approach are not well assessed.

A kinematic wave approximation has been also derived as an asymptotic limit of Richard's transport equation based on the assumption of a unit gradient of the total potential head (Sisson et al., 1980; Smith, 1983; Raats, 1983). This approximation applies during redistribution and drainage when the soil profile is draining freely. Both kinematic equations are derived from very different conceptual basis and the parameters involved are defined at different space and time scales. Whatever interpretation of these parameters, the underlying physical process unifying both approaches is the predominance of gravity driven flow over the dispersive capillary flow. The validity of these approximations and particularly the meaningful interpretation of model parameters require accurate experiments. Usually, problems arise when trying to measure flow variables and structural properties during rapid flow. Although sophisticated systems are implemented, the information obtained about the process is incomplete in most cases.

3.2.2 Transport in Soils with continuous or successively nested length scales

The hydraulic behavior varies in principle across void sizes. There is experimental evidence demonstrating that the boundary and initial conditions determine the degree of participation of the different pore classes in total water transport. Any classification of the pore space based on two-dimensional size only is impractical from the point of view of hydraulic behavior. Classifications based on the static hydraulic behavior of pore classes (e.g., with respect to the hydraulic conductivity) may not be realistic due to the dependence of flow on boundary conditions.

A macroscopic observer will recognize holes of varying sizes, geometry and vertical connectivity. At the macroscopic scale, heterogeneity and instabilities during the flow, i.e. different degrees of preferential flow may be observed. It has been shown (Levy, 1988; Ene, 1990) that the validity of Darcy's law is recovered by conveniently increasing the observation scale. But, scaling-up from the macroscopic to a megascopic scale is not practical. A megascopic REV sufficiently large to integrate the effects of macro-heterogeneity is required. A suitable REV would probably extend over several meters. Even if it would exist, it will be difficult to determine meaningful megascopic transport coefficients.

4. BIO-GEOCHEMICAL TRANSFORMATIONS AND SOIL HETEROGENEITY

Bio-geochemical transformations in the soil include various biotic and abiotic processes. They deal with C and N cycles (Mariotti, 1982), including the degradation of xenobiotic organic compounds, and the evolution of mineral compounds such as S, P and metals (Pankow, 1991), among other transformations. Their practical concerns deal with pollutant evolution in the soil, their fluxes at the interfaces with the underground, the underlying aquifers (Guillemin and Roux, 1991) and the atmosphere (Renault et al., 1997), ecotoxicology (Ramade, 1992), as well as human health and crop production.

Combined with transport processes, biotic and abiotic production/consumption may induce heterogeneous distribution of chemical compounds in the soil, depending on the balance between transport and transformations. This may be emphasised by pre-existing heterogeneity, e.g. heterogeneity in soil structure and substrate distribution (especially fresh organic residues). Finally, biological activities can modify transport properties of the porous media by different ways, e.g. the clogging of pores by micro-organisms and exocellular polymers, and the modification of the pore space structure by fauna activities.

Model that are relevant to describe the transport of reactive compounds in the soil, can greatly differ from models devoted to the same compounds in non-reactive porous medium. Differences go beyond the alone combination of biogeochemical transformations to transport: it may be required to describe transport at spatial scales non-relevant for non-reactive medium.

4.1 Biogeochemical Transformations Depend on Physico-Chemical Characteristics of the Soil

Biogeochemical transformations in the soil include biotic and abiotic ones. Biotic transformations mainly results from microbial activities (bacteria, fungi, microfauna), and root system consumption / production. Abiotic transformations includes reactions in the soil solution (acid/base, reduction/oxidation and complexation reactions), dissolution/precipitation and adsorption/desorption reactions. Similar transformations may originate simultaneously from biotic and abiotic processes. This is for example the case for the reduction of metals in anaerobic conditions, which tends to equilibrate their species with the couple (pH, reduction-oxidation potential) (Pankow, 1991), and result from microbial activities as electron acceptors for their energy supply (Watanabe, 1985). Biotic and abiotic transformations can modify locally the physical-chemical properties of the soil, when transport processes are not enough to minimise the product/substrate gradients, which are induced by such transformations.

Microbial transformations are generally reduction-oxidation transformations intended to supply energy to micro-organisms in order to maintain their life and, in favourable conditions, enable the growth of microbial communities. Other microbial transformations are devoted to the production of compounds constitutive of the microbial biomass. Similar transformations may thus appear in different conditions, either for energy supplying or the production of constitutive organic compounds: this is for example the case for NO_3^- which may be reduced to NH_4^+ through an assimilatory pathway in aerobic conditions - and then consumes energy - (Mariotti, 1982), or through a dissimilatory pathway as an alternative electron acceptor to O_2 (Fazzolari et al., 1990). This is also the case for CO_2 , which may be used either as an electron acceptor in severe anaerobic conditions leading to the production of CH_4 (Watanabe, 1985), or as a source of C to build organic materials in aerobic conditions, e.g. for autotrophic nitrifiers (Grant, 1995). The main electron acceptor is O_2 in aerobic condition. In anaerobic conditions, it vary in the following order with decreasing the reduction-oxidation potential: NO_3^- and NO_2^- , Mn^{4+} (MnO_2), Fe^{3+} (FeOOH), SO_4^{2-} , CO_2 (Watanabe, 1985), although Fe and Mn do not directly contribute to supply energy to microorganisms (Zehnder and Stumm, 1994). The electron donor is organic matter for heterotrophic organisms, the ability to use specific compounds highly depending on the metabolic pathways and the microbes themselves. Autotrophic bacteria may synthesise constitutive organic compounds by using only mineral ones.

As a consequence, microbial transformations depend on the availability of substrates. Models generally describes transformations by using Michaelis Menten formalisms adapted to enzymatic chemistry (Costes, 1978). To account for microbial dynamics, which indirectly affect the level of active enzymes, the growth of microbial community is often modelled using Monod formalism (Grant, 1995). Substrate consumption is then devoted to microbial maintenance and growth. May be some substrate released due to microbial death. Mathematical formalisms used to describe the effect of the substrate availability and physicochemical characteristics of the soil have generally to be regarded as empirical ones, although initially justified by theoretical assumptions. The pH and Eh conditions may affect the energy, which is required for or supplied by the transformation: as an example, reducing N_2 into NH_4^+ in aerobic conditions would consume too energy and this fixation appears mainly in anaerobic conditions, either in the anaerobic centres of nodules of leguminous plants (e.g. alfalfa), or in medium where anaerobic conditions prevail (Fazzolari et al., 1990). Physicochemical characteristics of the system may affect the chemical permeability of microbial walls and thus affect the actual substrate concentration at the enzyme level. Competition between metabolic co-existing pathways may be modified by the presence of substrate more favourable to one of them. At least, chemical compounds affect directly the enzyme activity; inhibition schemes have been proposed and are widely used (Costes, 1978), and biochemical transformations can also be stimulated by changes in the soil chemical characteristics.

To summarize, biogeochemical transformations in soils highly depend on its aeration status - which induce either aerobic or anaerobic transformations -, and the reduction-oxidation potential which affects the dominating anaerobic processes. The main other physical-chemical property affecting biogeochemical transformations is the pH of the soil solution. Biotic and abiotic transformations are closely linked. Unfortunately, one of the main gaps in the knowledge on soil biogeochemistry deals with the description of the interrelationships between microbial and physical-chemical transformations in soil. As an example and to our knowledge, no mechanistic model presently describes Eh evolution over paddy rice fields by simultaneously accounting for main microbial processes and physical-chemistry of the soil.

4.2 Biogeochemistry as Affected by, and Inducing Soil Heterogeneities

4.2.1 *Transient Unbalance between Transport and Production/Consumption*

Dealing with the aeration status and the pH of the soil, O₂ and CO₂ transport in the soil are of first concerns. As soon as the soil is wet enough, O₂ concentration may go down from nearly atmospheric concentration to zero value, through a few mm of saturated soils (Sexstone et al., 1985; Rappoldt, 1992; Sierra et al., 1995; Parry, 1999, among others) (Fig. 1). This results from the reduced diffusion of O₂ in water (about 10⁻⁴ times its value in air) and solubility (about 0.034 at 20°C): combined with classical O₂ microbial consumption rates in soil, anaerobic conditions may appear in saturated soil clods, when their radius exceed a value around 3 to 7 mm (Sierra and Renault, 1996).

Microbial activity may be high around fresh organic materials or particulate organic matters, soil), enabling anaerobic conditions to appear when a thin layer of water or saturated soil cover them (Parkin, 1987; Rappoldt, 1992; Parry, 1999). In practice, anoxic conditions appear as numerous anaerobic micro-sites in a soil, as soon as its water saturation exceeds a threshold around 50-60%. In this range of water content, there is no [O₂] vertical gradient in the air-filled macro-pore space: it can be observed only when the soil saturation exceed values around 85-90% (Renault and Sierra, 1994). Therefore, the description of O₂ distribution is relevant either only at the micro-scale, or simultaneously at microscale and soil profile scale, or at the soil profile scale only, depending on the range of the soil water saturation and the structure of the porous medium. Scales of interests would greatly differ for gases, from which the production and consumption are not greatly affected by the soil: as a first approximation, this would be the case for ²²²Rn distribution in soils, which first depends on vertical diffusion and convection only (Pinault and Baubron, 1997).

Main conceptual differences between O₂ and CO₂ distributions in soils results from the facts that (i) CO₂ is produced by different metabolic pathways, including anaerobic ones, (ii) CO₂ is consumed by

autotrophic bacteria, and (iii) $[\text{CO}_2]$ in the soil solution is greatly affected by dissociation and complexation reactions. As a consequence, the $[\text{O}_2]$ to $[\text{CO}_2]$ gradient ratio in saturated soil zones generally increase with the pH of the soil solution, and is about 1 in the air-filled pore space, although it is affected by the respiratory quotient of the soil and the interdependency between gas transport in the air-filled pore space (Freijer and Leffelaar, 1996).

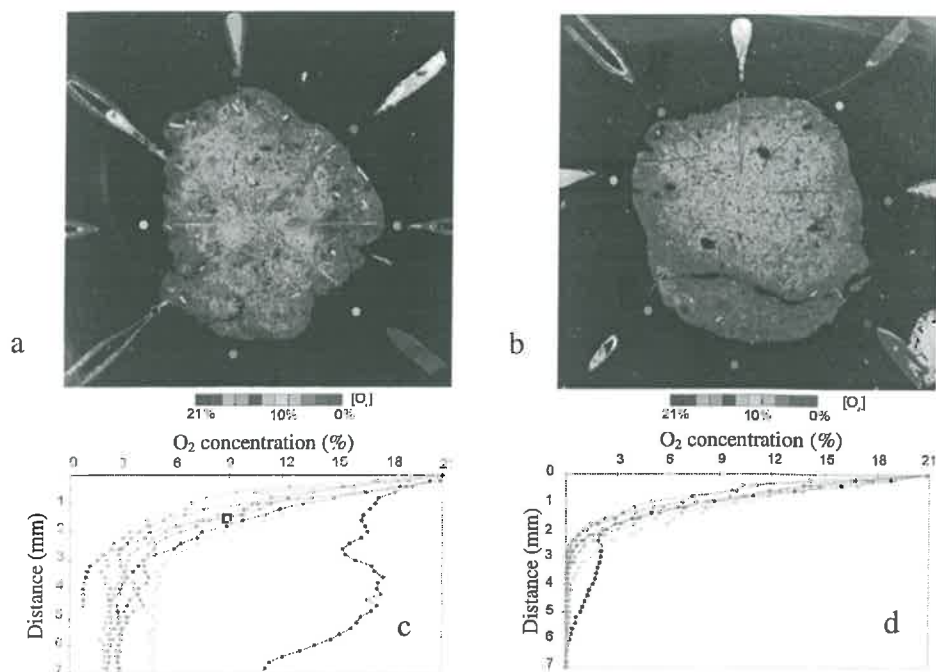


Figure 1: Thin sections from clods of a pasture (a) and a cropped (b) soil, where 8 $[\text{O}_2]$ profiles were recorded (c and d), at a -1 kPa water suction (from Parry, 1999).

Many other substrates/products are subject to gradients in their spatial distribution: they include (i) NO_3^- produced by nitrification, absorbed by plant roots and reduced in anaerobic conditions in N_2O , N_2 and/or NH_4^+ , and (ii) soluble organic compounds, which are produced by decomposition of insoluble organic matter and exuded by roots.

As a conclusion, biogeochemical activities may induce gradients of substrates and other physical-chemical properties. In these conditions, biogeochemical activities can not be easily linked to the bulk concentration of substrate in the soil. One of the major consequences of these sources/sinks is to modify the distribution of substrates in space and to imply a description of combined transport-reaction processes over spatial scales and directions, which would be out of interest for non-reactive porous media.

4.2.2 Pre-existing Heterogeneity and their Effect on the Soil Behaviour

Pre-existing heterogeneities deal with the soil transport properties (see preceding sections) and the distribution of the substrates which are little subject to transport and affect biogeochemical transformations. Organic materials are among the main substrates sustaining these 2 preceding characteristics. Their spatial distribution results partly from the root growth and the incorporation of residues in the soil. They include soluble and non-soluble materials. We focus here on (i) soluble organic compounds exuded by the roots and (ii) non-soluble ones, because there is generally a correlation between total and soluble organic matter contents in the soil (Burford and Bremner, 1975).

Microbial activities are generally all the more important as organic materials have been recently incorporated in the soil, although its chemical composition affects microbial activity. As an example, Parkin (1987) showed that a single fresh plant residue could be responsible for 25 to 85% of the denitrification in decimetric soil cores (Fig. 2). Simulating the spatial distribution of those hot-spot of denitrification and random process of soil core sampling, Parkin (1987) obtained a simulated distribution in core denitrification rates nearly similar to the experimental one.

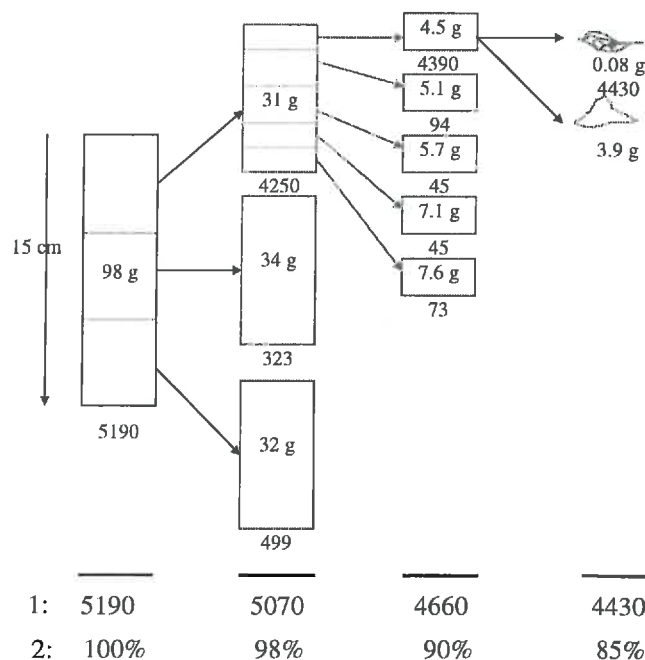


Figure 2: Identification of active denitrifying sites in soil by a core segmentation (Parkin, 1987)

Similar observations have been performed by Christensen et al. (1990). Older organic materials cannot be neglected: Parry et al. (1999b) noted that particulate organic matters could explain about half of the denitrification of cropped soil clods.

Other heterogeneities in organic matter distribution in the soil results from the organic matter exuded from the root system. They induce high microbial activities in the first mm around the root. For example, Bidet et al. (1999a and 1999b) measured root O_2 consumption for root in initially sterilised Agar gel. Although the gel was treated by a bactericide and a fungicide, they observed microbial activities in the 300 μm around the root, which may reach 100 times microbial respiration in current soils.

4.2.3 Fed-back Effects of Biogeochemical Activities on Soil Transport Properties

Biogeochemical activities can affect soil transport properties, either by modifying the pore space properties, or modifying the fluid properties in the case of liquid water (e.g. by synthesising mucilage in anaerobic conditions). Heterogeneities in soil transport properties induced by biogeochemical processes are the clogging of pores by bacterial films with extracellular polymers (Taylor and Jaffé, 1990; Vandevivere and Baveye, 1992), gas and liquid transport within the roots, and the effects of the mesofauna on the pore space structure.

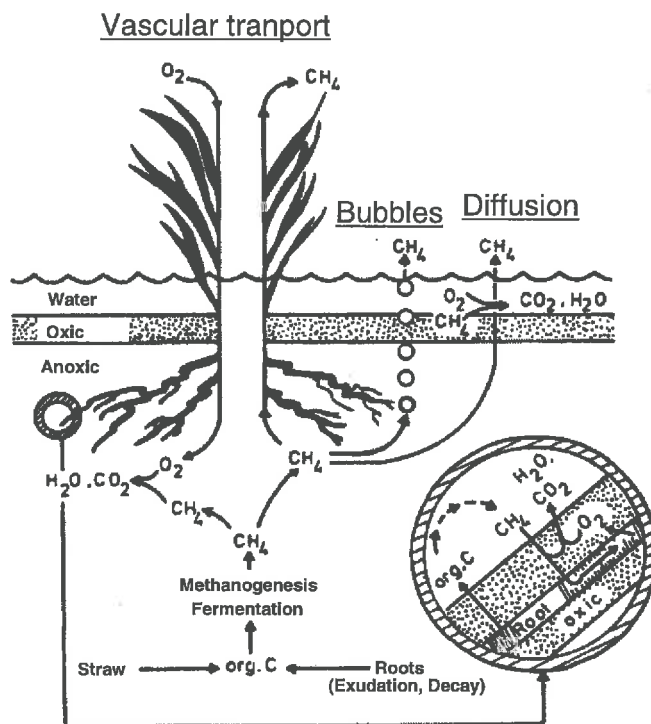


Figure 3: production, transport and consumption of CH_4 in flooded paddy rice field
(from Conrad, 1989).

For example, root systems of plant adapted to flooded soils (e.g. rice, papyrus) develop a lacunar intercellular space – the aerenchyma – which is devoted to gas transport from shoots to roots (and inversely) (Drew and Fourcy, 1986; De Willigen and Van Noordwijk, 1984; Van Noordwijk and De Willigen, 1984). It enable to supply O_2 to the root and the soil close to the root (Visser et al., 1997), and may be the main pathway for CH_4 emitted to the atmosphere (Seiler, 1984). For this gas, the production is partly counterbalanced by its consumption in oxic layers of the soil, i.e. the soil surface and thin layers of soil surrounding the roots. Nevertheless, roots acts in various sometimes counterbalancing ways, and it is not easy to quantitatively describe their effect on the rhizosphere.

The pore space structure is affected by roots and fauna activity. As an example, worms burrows results from different ecological types of earthworms (Bouché, 1977): whereas epigeic worms live at the soil surface, anecic and endogeic worms live in the soil. Anecic worms consume organic matter at the soil surface, and burrow nearly vertical and poorly connected holes, which may be some meter long (Kobel-Lamparsky and Lamparski, 1985). Endogeics worms consume organic matter in the soil, and burrow networks of macropores, which direction in space are various. Worm burrow systems vary with time: they result from the balance between burrowing and backfilling with casts (Fig. 4).

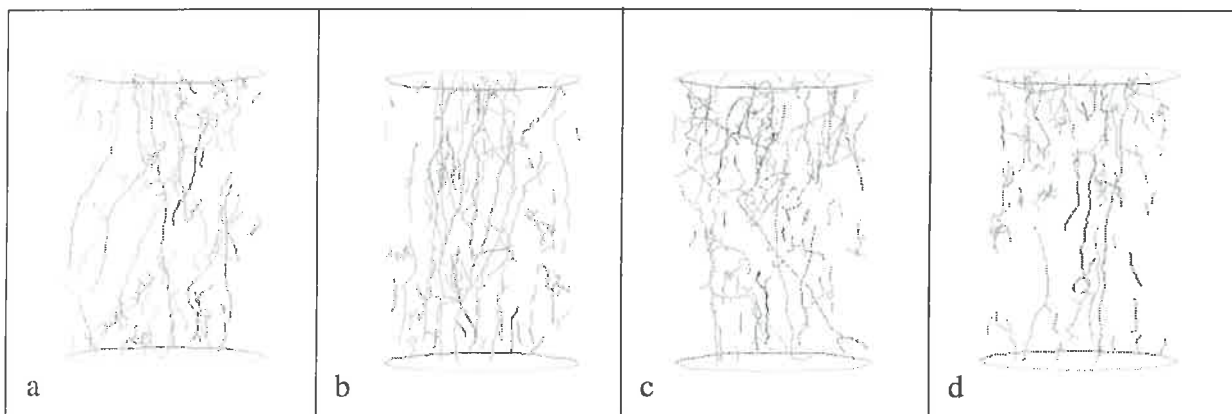


Figure 4: Seasonal variations in 3D burrow system resulting from earthworm activity in a Switzerland pasture soil (from Capowiez et al., 1998). a and b: spring; c and d: fall.

Agricultural soil management affect the number of worms per m^2 (about 500 in pasture soil and less than 100 in cropped soils; Lee, 1985), and their biodiversity (anecic and epigeic worms are highly sensitive to the destruction of burrow holes and the decrease in the soil organic matter content; Edwards and Lofty, 1982), leading to a change in the characteristic features of burrow hole networks.

Only a few works deal with burrow hole effect on transport properties. The highest observed effects deal with burrow holes of anecic worms on water bypass flow (Bouma et al., 1982; McCoy et al., 1994). Some other works deal with the effects of burrow holes on gas diffusion in compacted soils (Kretzschmar and Monestiez, 1992).

4.3 Accounting for pre-existing and induced soil heterogeneities in models

Because modelling biogeochemical transformations needs to combine transport and biogeochemical processes simultaneously at different scales, modelling the resulting behaviour of the soil is a challenge. We don't pretend to give an overview of practical solutions to so great and various difficulties. If practical solutions are already in use for well-defined problems, to our opinion, combining transport to biogeochemical processes in models constitutes a great field, which still remain poorly explored.

5. CONCLUSION

The soil is a porous medium, where transport and biogeochemical transformations simultaneously take place. Improving our knowledge on soil main properties is justified by its importance in agricultural productions, and its environmental concern as a reactive interface with the underground (and the contained water resources), and air (on which a lot of researches have recently focused on the composition dealing with greenhouse gases, O₃ and acid chemicals).

Mass (water, solutes, gases and solid particles) and heat transports are affected by properties specific to the soil :

- the soil is continuously deformed by climatic (e.g. swelling-shrinking due to moisture changes), biological (e.g. macropores network burrowed by earthworms) and human events (e.g. soil tillage) and local soil transport properties can be modified by microscopic changes such as the clogging of pores by biofilms such as "bacteria-extracellular polymers" or solid particles. These processes may result in a soil structure, where heterogeneities have to be accounted for at different spatial scales;
- biogeochemical transformations in the soil induce heterogeneities in substrates and products distributions, leading to describe transport of these compounds at spatial scales which would be non-relevant for transport of the same compounds in less reactive media;
- spatial scales of interests range from microscopic scales (e.g. to describe colonisation of fresh plant residues and decomposition by fungi, bacteria ..., and to describe anoxic microsites in

saturated clods) to meso-scale (e.g. to watersheds). Several intermediate scales may be defined including soil cores and the soil profile scales. One of the main conceptual limit of this scale is the often 1D description of the soil behaviour. Indeed, it is now well recognized that many processes need a multi-dimensional description to be relevant (e.g. water absorption by the root system, preferential infiltration of water, O₂ transport).

There is still a need of improving our knowledge in several domains:

- basic processes, including the description of transport (preferential infiltration, runoff, solid transport);
- interrelationships between processes of various natures and their feedback effects, including interactions between transport and biogeochemical processes;
- the modelling of the basic processes, and their interrelationships in the soil, including simplified approaches to be relevant for practical concerns.

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