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Transport modeling of pesticides in soil porosity using 3D maps provided from X-ray computed tomography

N.Elyeznasni(1), V.Pot(1), P.Garnier(1), L.Young(2), F.Sellami(3), I.Ginzburg(4) and P.Benoit(1)

1. UMR INRA - AgroParisTech, Environment and Arable Crops, BP01, 78850 Thiverval-Grignon, France (nelyeznasni@grignon.inra.fr/Phone: +33 1 30 81 54 02)
2. SIMBIOS, University of Abertay Dundee, Bell street, Dundee, DD1 1HG
3. INRAP, Grand Sud-ouest-Pessac, France
4. CEMAGREF, Antony Regional Centre, parc de Turvoie-BP44, 92163 Antony, France

The transport of reactive solutes in soils and aquifers plays an important role in a variety of fields, including leaching of agrochemicals from soil surface to ground water. Heterogeneities of physical (structure of soil), physico-chemical (adsorption/desorption) and biological origins do not appear explicitly in transport models of solutes in soils. Traditional mathematical models treat movement and sorption reactions in soils by implicit description of heterogeneities (non-equilibrium transport models: two-porosity, multiple-permeability, kinetic sorption). The identification of void space and simulation of reactive solute transport through it are a challenging task because of complicated geometry. In this work, we have constructed a modeling approach to describe reaction kinetics and dynamics of pesticides at microscopic scale compatible with pore organization. As a first step of our work we performed 3 dimensional maps to describe pore space and localize reactive sites in soil. This step is very important to study the transport of solutes in real geometry. The maps were obtained by scanning soil cores using X-ray computed tomography which is imaging by sections technique. To make a sectional image by X-ray tomography we have to move X-ray source in opposite directions during the exposure to make sharper plans. This technique is based on mathematical procedure called tomographic reconstruc-

tion. The soil cores (5 cm heigth and 5 cm diameter) were sampled in the surface horizon of a clay-loam soil provided from Feucherolles site (France). The sampling was performed after tillage that provided incorporation of fresh organic matter residues (wheat straws) in the surface horizon and was localized in the regions of high content of fresh organic matter. Resolution of the images was of 68 microns. Those tomograms have been explored as a serial of 750 surfaces by analyzing the Grey level of images. All surfaces were studied to detect different levels of density indicating different nature of soil constituents such as particulate organic matter, organo-mineral phase and void (porosity). We investigated also the pore space connectivity which is an important topological property of soil to model transport. The high quality of the tomographic images allowed to distinguish particulate organic matter from porosity and organo-mineral phases. Such a finding was further compared to two dimensional thin sections of close resolution (40 microns) of the same soil samples where void, fresh particulate organic matter and organo-mineral phases can be identified by micromorphological observations through optical microscopy. After localization of diverse heterogeneities in a 3D map, the transport of solutes will be studied at mesosocopic scale using lattice Boltzmann multi-relaxation-time model. This method, originated from lattice gases theory about fiftheen years ago, contrasts with the traditional approach to CFD models by adopting a bottom-up approach to fluid modeling. To achieve this, it describes a fluid at a molecular level and matches the Navier-Stokes equations as a second-order approximation of the exact microscopic mass and momentum conservation laws. Dropping the conservation of the momentum, the method is adapted for solving advection-diffusion equations and further extended in our work to describe (or include) also reaction kinetics by integrating the adsorption/desorption and degradation by laws of first order.