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Data set title: **Solid, air and water phase distributions of a UK sandy loam soil packed at five bulk densities, 2018**

Data overview: This data set provides 30 Computed Tomography (CT) based soil microstructures providing the distributions of soil, air and water. Two water conditions (20±0.5 and 80±0.5%, expressed as the volume ratio of visible pore space) for 5 soil bulk densities, 3 repetitions per bulk density (30 images). Each image will have a domain size of 512x512x512 voxels.

Soil microstructure images are named: "BDXX_R_SW.tif", with XX designating the bulk density (1.2, 1.3, 1.4, 1.5, 1.6 g cm^{-3}), R the repetition (1, 2 or 3) and SW the water saturation (20±0.5 or 80±0.5%) computed as described below. Each image holds 512 slices along the z direction and is saved as ".tif" image. Soil, water and air volume elements of the image are represented using a grayscale value of 255, 127, and 0, respectively.

Material and methods

Soil preparation

Soil samples used in this study originated from a sandy loam soil collected in 2011 at an experimental site, Bullion field, situated within the James Hutton Institute in Invergowrie, Scotland. The soil was air-dried and soil aggregates were sieved down to an aggregate size of 1–2 mm and stored in a cold room (4 °C). The physicochemical characteristics of the selected soil aggregate fraction (1–2 mm) are as follows: sand, 55.7%; silt, 31.0%; clay, 13.3%; organic matter, 5.5%; C/N ratio, 17.1. For the experiment, the soil was sterilized by autoclaving twice (moist heat) in glass bottles at 121 °C at 100 kPa for 30 min with a 24-hr interval time.

Preparation of soil microcosms

Soil microcosms were prepared in polyethene rings of size 3.4 cm^3 (inner diameter 17.0 mm and height 15.0 mm) packed at five soil bulk densities, 1.2, 1.3, 1.4, 1.5, and 1.6 g cm^{-3} . To ensure the air-filled pore space was the same of all treatments, the gravimetric water content ranged from 0.13, 0.11, 0.09, 0.07, to 0.06 for the bulk densities, respectively. Three replicates per treatment were prepared, producing 15 soil microcosms in total. Details of the preparation are provided elsewhere (Juyal et al., 2018, Front. Environ. Sci., 6:73).

Computed Tomography Imaging

The impregnated samples were scanned using a Metris X–Tek HMX CT scanner (NIKON Metrology, Tring, UK). Samples were scanned at 24 μm voxel resolution with energy settings of 105 keV and 96 μA and 2000 angular projections. A Molybdenum target with a 0.25-mm aluminium filter was used. Reconstruction of radiographs into 3D volumes was performed using Metris X-Tek software CT Pro v2.1 (NIKON Metrology). A volume processing software, VGStudio MAX V2.2 (Volume Graphics, Heidelberg, Germany), was used to change contrast in reconstructed volumes and to export image stacks (*bmp format) for further processing.

Image pre-processing

X-ray CT data was thresholded using an in-house-developed indicator kriging method published elsewhere (Houston et al. 2013, Computers & Geosciences, 54, 239–248). The unconnected solid particles of the thresholded images were removed using the Plugin 3D Fill holes of ImageJ (Ollion et al. 2013, Bioinformatics 29(14):1840-1).

Air-water distribution modelling

Water-air distributions corresponding to the target saturation levels, S_w, of 0.8 and 0.2 were obtained for the set of images using a two-phase single component two-relaxation times lattice-Boltzmann model (Ginzburg 2005, Adv. Water Resour, 28(11):1171-1195) parameterised as described by Genty and Pot (2013, Transp Porous Media, 96(2):271-294) to which the reader is referred for a definition of the symbols used here.

The independent parameter c_s^2, was set to 1/3, the eigenvalue, λ_e was fixed by an arbitrarily value of the kinematic viscosity, v = 1/6 along v = (1/3)Λ_{eo}, for the case of incompressible Stokes flow. The eigenvalue, λ_o was calculated from a fixed value of $\Lambda_{eo} = 3/16$.

We used G= −0.16 .and W= 0.15 for simulations with S_w=0.8 in order to match the fully-wetting fluid conditions (zero contact angle between liquid and solid phases). W was set to 0.13 for the simulations with S_w=0.2, expect for one of the images (BD16_3), where the value 0.125 was assumed.

Bounce-back conditions were applied at solid boundaries. Since some pores were cut by the edges of our images, we applied hydrophobic conditions (W = 0) at the boundary voxels that contained air in the CT data in order to simulate realistic liquid–gas distributions. Hydrophilic conditions (W > 0) were applied elsewhere.

Initial density of water particles in the image (P_I) was computed for each different saturation level from the mass balance equation:

$$\mathrm{P}_I = \left((\rho_l - \rho_g)S_{w0} + \rho_g\right)\ \phi\ I_s$$

where ρ_g and ρ_l are the density of the gas and liquid phases (ρ_g =0.03 mu lu^{-3} and ρ_l = 2.42 mu lu^{-3}), respectively, S_{w0} is the water saturation index of the segmented CT image, ϕ is the void porosity and I_s the size in voxels of the image. P_I was distributed in the pore space in a two steps way. All pore space sites were first initialized with a density ρ_g. The remaining water particles ($\mathrm{P}_I - \rho_g \phi I_s$) was then uniformly distributed in the two layer of voxels neighbouring the solid voxels of the segmented CT images.

We developed an iterative searching algorithm on S_{w0}. The iterative procedure, uses a double loop to find a first, approximate solution for S_{w0} before entering the final, and more time consuming, main iterative loop. Time lengths of the lattice-Boltzmann loop of the warm up and main iterative loops were set, respectively, to 2,000 and 10,000 lattice-Boltzmann time units and the tolerance level was set to 0.005 (±0.5%). The water density predicted by the TRT-LBM was thresholded using the mean value of ρ_g and ρ_l, 1.225. The simulations were run in computed nodes having two Intel E5-2620 v4 (Broadwell) CPUs under a Red Hat Enterprise Linux Server release 7.2 (Linux Kernel version 3.10.0).

Data set images

Each microstructure holds 512 slices along the z direction and is saved as ".tif" image. Each volume element (voxel) is explicitly assigned to soil, water or air following the procedure described above. Soil voxels have a value of 255, water voxels have a value of 127, and air voxels have a value of 0.