SOIL

Discussions

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Interactive comment on "Quantitative imaging of the 3-D distribution of cation adsorption sites in undisturbed soil" *by* Hannes Keck et al.

Anonymous Referee #2

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This is a very interesting study determining the spatial distribution of cation adsorption sites in undisturbed soil columns. Until now, our knowledge about the spatial heterogeneity down to the millimetre scale (and smaller) of this important soil property is very limited and quantitative approaches are strongly needed. The authors compared a 3-D quantitative imaging approach to determine the cation exchange capacity with a conventional method. In general the manuscript is of high quality and well written. I have just a few comments related to the methodological approach including one suggestion for a preliminary test (small amount of work).

Introduction: The list of references on current X-ray CT studies (page 2 line 25 to page 3 line 18) is limited on what seems to be a subjective selection by the authors, but that cannot be hold against them as the field is growing quickly and it is neither possible nor

desirable to reach a comprehensive overview here. The references are all up to date!

Methods: Page 4, line 8: Please add a reference for the ammonium acetate method you used. Page 4, line 14: You referred to the "loss of ignition method" for the analyses of carbon in your soils but you used a CNS analyser. Please check / clarify. page 4 line 23: "inverted" should be replaced by "reconstructed into 3-D tomograms"

Reference gray values for Al, K and Ba in the contrast image (Fig. 1): What was the motivation to use different concentration for the two solutes (0.1M KCl vs 0.3M BaCl2)? Why did you keep the remaining volume inside the soil column air-filled? In a more realistic scenario it should be filled with dry soil at the same or at least the average bulk density of all investigated samples to mimic the X-ray attenuation by the soil matrix. For instance, the reference gray value for KCl will be below 16225 if pure KCl was detected inside soil, because the photon flux will already be attenuated during the passage of the soil matrix, and it is difficult to estimate by how much. I would strongly advice to do such a preliminary test with the same solution columns surrounded by differently packed soil that covers the range of bulk densities reported in Table 2, analyse the effect on the reference gray values of the different materials and add this information as supplementary material. The amount of work to do this is small. If the changes turn out to be small, then you can use this as an asset of your approach to use polychromatic X-rays to measure cation adsorption sites. As this is really the first study in this respect it should lay out the foundations as thoroughly as possible. Additional information about the interplay between attenuation of polychromatic X-rays in water and the soil matrix can be retrieved e.g. in Weller et al. (2017).

Page 6 line 11: To my knowledge an affine transformation cannot account for local deformations, but only for a change in position and perhaps global distortion of the sample.

Page 6, relationship between gray values and barium mass: It is not clear to me, also after consulting Koestel & Larsbo (2014), how Cmax is determined. Is it the hypothet-

ical mass of Ba in one voxel assuming 0.3M BaCl is reached in a pure pore voxel, i.e. no partial filling of that voxel with the solid phase? Also, readers might wonder how changes in background porosity might influence the interpretation of the estimated BaCl2 mass. Does the same increase in m (BaCl2 mass) always result in the same increase in gamma (gray value), no matter whether a voxel is partially filled with pores by, say, 30% or 70%?

Page 6-7, Spatial distribution of cation exchange capacity: In order to estimate CEC from m, you need to know the mass of soil in the two regions of interest (soil matrix vs. macropore walls). Do you estimate the (fluctuating) mass of soil per voxel and cumulate this over all voxels in the respective regions?

Table 1: Please indicate sampling depths and soil horizons for all soils you used

References: Weller, U., F. Leuther, S. Schlüter, H.-J. Vogel: Quantitative analysis of water infiltration in soil cores using x-ray, Vadose Zone Journal (in press), url: https://dl.sciencesocieties.org/publications/vzj/first-look

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