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Microscale soil structure development after glacial retreat – using machine-learning based segmentation of elemental distributions obtained by NanoSIMS

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Soil organic matter (SOM) is distributed on mineral surfaces depending on physicochemical soil properties that vary at the submicron scale. Nanoscale secondary ion mass spectrometry (NanoSIMS) can be used to visualize the spatial distribution of up to seven elements simultaneously at a lateral resolution of approximately 100 nm from which patterns of SOM coatings can be derived. Existing computational methods are mostly confined to visualization and lack spatial quantification measures of coverage and connectivity of organic matter coatings. This study proposes a methodology for the spatial analysis of SOM coatings based on supervised pixel classification and automatic image analysis of the ^{12}C, $^{12}C^{14}N$ (indicative for SOM) and ^{16}O (indicative for mineral surfaces) secondary ion distributions. The image segmentation of the secondary ion distributions into mineral particle surface and organic coating was done with a machine learning algorithm, which accounts for multiple features like size, color, intensity, edge and texture in all three ion distributions simultaneously. Our workflow allowed the spatial analysis of differences in the SOM coverage during soil development in the Damma glacier forefield (Switzerland) based on NanoSIMS measurements (n=121; containing ca. 4000 particles). The Damma chronosequence comprises several stages of soil development with increasing ice-free period (from ca. 15 to $>$700 years). To investigate mineral-associated SOM in the developing soil we obtained clay fractions ($<$2 μm) from two density fractions: light mineral (1.6 to 2.2 g cm^3) and heavy mineral ($>$2.2 g cm^3). We found increased coverage and a simultaneous development from patchy-distributed organic coatings to more connected coatings with increasing time after glacial retreat. The normalized N:C ratio ($^{12}C^{14}N$: ($^{12}C^{14}N$ + ^{12}C)) on the organic matter coatings was higher in the medium-aged soils than in the young and mature ones in both heavy and light mineral fraction. This reflects the sequential accumulation of proteinaceous SOM in the medium-aged soils and C-rich compounds in the mature soils. The results of our microscale image analysis correlated well with the SOM concentration of the fractions measured by elemental analyzer. Image analysis in combination with secondary ion distributions provides a powerful tool at the required microscale and enhances our mechanistic understanding of SOM stabilization in soil.