EGU23-12421, updated on 04 Mar 2024
https://doi.org/10.5194/egusphere-egu23-12421
EGU General Assembly 2023

Quantifying the impact of 3D pore space morphology on diffusive mass transport in loam and sand

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Effective diffusion is an important macroscopic property for assessing mass transport in porous media. Numerical computations on segmented 3D CT images yield precise estimates for diffusive properties. On the other hand, geometrical characteristics of pore space like, e.g., porosity, specific surface area and further transport-related descriptors can be easily computed from 3D CT images and are closely linked to diffusion processes. In the present contribution, we consider six different soil samples of loam and sand, whose 3D microstructure is quantitatively investigated using univariate as well as bivariate distributions of geometrical descriptors of pore space. This information is used for investigating microstructure-property relationships by means of empirically derived regression formulas, where a particular focus is put on the differences between loam and sand samples. In this way, it is possible to obtain a deeper understanding for the relationship between the 3D microstructure of the pore space and the resulting diffusive properties due to the analytical nature of the prediction formulas. In particular, it is shown that formulas existing so far in the literature for predicting soil gas diffusion can be significantly improved by incorporating further geometrical descriptors such as geodesic tortuosity, chord length distribution or constrictivity. The robustness of these formulas is investigated by fitting the regression parameters on different data sets as well as by applying the empirically derived formulas to certain data that is not used for fitting. Among others, it turns out that a prediction formula based on porosity as well as mean and standard deviation of geodesic tortuosity performs best with regard to the coefficient of determination and the mean absolute percentage error. Moreover, it is shown that with regard to the prediction of diffusive properties the concept of geodesic tortuosity is superior to geometric tortuosity, where the latter is based on the skeleton of the pore space.