

Effective structural descriptors for natural and engineered radioactive waste confinement barriers

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The microstructure of a radioactive waste confinement barrier strongly influences its flow and transport properties. Numerical flow and transport simulations for these porous media at the pore scale therefore require input data that describe the microstructure as accurately as possible. To date, no imaging method can resolve all heterogeneities within important radioactive waste confinement barrier materials as hardened cement paste and natural clays at the micro scale (nm-cm). Therefore, it is necessary to merge information from different 2D and 3D imaging methods using porous media reconstruction techniques.

To qualitatively compare the results of different reconstruction techniques, visual inspection might suffice. To quantitatively compare training-image based algorithms, Tan et al. (2014) proposed an algorithm using an analysis of distance. However, the ranking of the algorithm depends on the choice of the structural descriptor, in their case multiple-point or cluster-based histograms.

We present here preliminary work in which we will review different structural descriptors and test their effectiveness, for capturing the main structural characteristics of radioactive waste confinement barrier materials, to determine the descriptors to use in the analysis of distance. The investigated descriptors are particle size distributions, surface area distributions, two point probability functions, multiple point histograms, linear functions and two point cluster functions. The descriptor testing consists of stochastically generating realizations from a reference image using the simulated annealing optimization procedure introduced by Karsanina et al. (2015). This procedure basically minimizes the differences between pre-specified descriptor values associated with the training image and the image being produced. The most efficient descriptor set can therefore be identified by comparing the image generation quality among the tested descriptor combinations. The assessment of the quality of the simulations will be made by combining all considered descriptors. Once the set of the most efficient descriptors is determined, they can be used in the analysis of distance, to rank different reconstruction algorithms in a more objective way in future work.

Karsanina MV, Gerke KM, Skvortsova EB, Mallants D (2015) Universal Spatial Correlation Functions for Describing and Reconstructing Soil Microstructure. PLoS ONE 10(5): e0126515. doi:10.1371/journal.pone.0126515

Tan, Xiaojin, Pejman Tahmasebi, and Jef Caers. "Comparing training-image based algorithms using an analysis of distance." *Mathematical Geosciences* 46.2 (2014): 149-169.