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Characterization of spatial heterogeneity of geomaterials in large scale groundwater bodies through a compositional data approach

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Characterization of the spatial distribution of geomaterials and of the associated attributes is a key step associated with the set up of a hydrogeological model. Geological information are often used as a basis for this purpose. One of the most common sources of geological information is provided by available borehole data. However, geological and hydraulic information are often available at different scale. In most cases hydraulic parameters are only measured at point locations, e.g. based on pumping test, which cannot be directly transferred into 3D large-scale parameter fields. However, in some regions even geological information are scare. In such situations, information about aquifer facies and material groups need to be interpolated and serve then as a base to derive key hydraulic parameters, such as hydraulic conductivity, or transport parameters, such as porosity, diversity or reactive surfaces. Sedimentary descriptions are usually achieved when drilling a borehole. Classification of sediments rests on a well defined procedure and provides a preliminary assessment on particle size distributions of the samples analyzed. Based on sedimentary descriptions of the boreholes we construct synthetic particle size distribution curves. These particle size distribution curves can be used to calculate major local attributes of the system (e.g., hydraulic and some specific transport parameters). Based on these types of readily-available information this study aims at developing a procedure to assist construction of a high resolution geological model suitable to be transferred into a flow and transport model that is then used for water resources management issues. We therefore aim to estimate storage and transmissivity with a high reliability by accounting for the material composition in the interpolated space. We rely on a compositional data analysis framework and represent particle size fractions associated with a given location as a compositional vector. These vectors are then projected onto a computational grid through compositional kriging to characterize the spatial heterogeneity of the system. We compare these results against an approach that is based on clustering the ensuing information to obtain distinct geomaterial classes and then assess their spatial distribution through indicator kriging. After the 3D field of grain size distribution curves is generated, they are transferred into hydraulic parameter. Although the process of clustering and using material classes is inevitably associated with a loss in information the procedure of forming a representative particle size distribution around the compositional clusters attempts to keep this loss of information at a minimum. The benefit of interpolating the compositional data instead of directly interpolating inferred parameters is that the particle size distribution curves contain a huge set of information from hydraulic to transport and reactive parameters, which would be lost using hydraulic

conductivity exclusively, while the use of material classes increases the efficiency of the calibration of the groundwater model.