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## Using geological entropy to support the optimization of coupled pump-and-treat systems in contaminated heterogeneous aquifers

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Aquifers are heterogeneous systems with limited accessibility for their characterization. Their hydrogeological parameterization is therefore complicated, producing uncertainty in groundwater and solute transport modelling. When numerical models are used to support pump-and-treat (P&T) applications to control the migration of solute plume in heterogeneous aquifers, the uncertainty in the design of the array of boreholes forming the hydraulic barrier and in the calculation of optimal pumping rates (Q) strongly depends on the variability in aquifer properties such as the hydraulic conductivity (K) (e.g. Bayer et al. 2004).

Geological entropy (Bianchi and Pedretti 2017, 2018) is a new approach that combines multiple controls of flow and solute transport in heterogeneous media. Geological entropy relies on the assumption that flow and transport are correlated to the degree of spatial order in the heterogeneous aquifer structure, which is measured by metrics derived from the information entropy concepts. Geological entropy is particularly useful to detect and highlight structural differences in aquifers associated to the presence of extreme connected features, such as fractures (Pedretti and Bianchi, 2019) or connected high-K facies (Bianchi and Pedretti 2017, 2018).

In this work, we present the result of an application of geological entropy to support the optimization of P&T scenarios in heterogeneous aquifers. A numerical case study based on the stochastic analyses by Bayer et al (2004) was reevaluated and extended. Multiple P&T setups considering both hydraulic and physical barriers were evaluated using stochastic geostatistical modeling based on 2D Sequential Gaussian Simulations and particle tracking simulations. The goal of Bayer et al (2004) was to identify the best hydraulic and physical barriers combination minimizing Q that allow for fully controlling a plume migrating in the aquifer.

In our work, we maintained a similar setup and optimization criteria, yet different aquifer structures using Sequential Gaussian and Indicator Simulations and model dimensionality (2D vs 3D simulations) are assessed. By doing this, we tested if the behavior of aquifer structures and connectivity among K clusters plays a role in defining Q, and if geological entropy can be used as the approach to disentangle the differences among the tested scenarios.

The results suggested that optimal pumping rates are very sensitive to the aquifer structures and model dimensionality. In particular, the range of variability of optimal Q is strongly reduced for

systems characterized by shorter entropic scales, which means short-scale continuity of the spatial order of K patterns. 3D systems imply more percolation, connection among K clusters, enhancing mixing and homogenizing better the system dynamic properties.

It is thus concluded that the selection of the optimal P&T configuration is strongly sensitive to the tested variables, and that geological entropy provides a potential geologically-based tool to support decision makers when defining the optimal (i.e. cost-effective) implementation of coupled P&T systems.

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**How to cite:** Pedretti, D. and Bianchi, M.: Using geological entropy to support the optimization of coupled pump-and-treat systems in contaminated heterogeneous aquifers, EGU General Assembly 2020, Online, 4–8 May 2020, EGU2020-20560, https://doi.org/10.5194/egusphere-egu2020-20560, 2020