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EXECUTIVE SUMMARY OF THE THESIS

Data-Driven Enhancement of Ordinary Kriging for Uncertainty-Aware Aquifer Characterization in Thermal Energy Storage Systems

LAUREA MAGISTRALE IN ENERGY ENGINEERING - INGEGNERIA ENERGETICA

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1. Introduction

Aquifer Thermal Energy Storage (ATES) has emerged as a promising technology for seasonal energy storage because it enables the storage and recovery of thermal energy within natural aquifers, thereby supporting the integration of renewable energy sources and reducing greenhouse gas emissions [1, 4]. The performance of an ATES system strongly depends on the hydraulic conductivity distribution of the aquifer, which governs groundwater flow and heat transport [3]. However, hydraulic conductivity can only be measured at limited borehole locations, making its spatial characterization a major challenge in groundwater modelling [3].

Ordinary Kriging (OK) is one of the most widely used geostatistical techniques for spatial interpolation of hydraulic conductivity because it exploits the spatial correlation among observations to estimate values at unsampled locations [3]. In the present study, OK prediction is assumed to provide an estimator of the unknown hydraulic conductivity. Within a Maximum Likelihood framework, the discrepancy between the observed hydraulic conductivity and the corresponding cross-validation prediction is interpreted as an estimation error that can sub-

sequently be modelled using machine-learning techniques.

Based on this framework, two hybrid geostatistical-machine learning approaches are investigated by combining OK with Random Forest (OK-RF) [2] and Gaussian Process Regression (OK-GPR) [7]. Four hydraulic conductivity representations are considered: (i) a homogeneous reference field, (ii) a deterministic OK field, (iii) a hybrid OK-RF field, and (iv) a hybrid OK-GPR field. These hydraulic conductivity fields are subsequently incorporated into a three-dimensional coupled groundwater flow and heat transport model developed using MATLAB Reservoir Simulation Toolbox (MRST) [6] to investigate how different hydraulic conductivity representations influence the predicted thermo-hydraulic response of an ATES system under identical operating conditions.

2. Methodology

2.1. Hydraulic Conductivity Characterization

Proposed methodology combines classical geostatistics with machine learning (ML) to gener-

ate alternative hydraulic conductivity representations for numerical groundwater flow and heat transport simulations. OK was first applied to interpolate the logarithm of hydraulic conductivity ($\log K$) based on the spatial correlation structure described by an experimentally fitted exponential variogram model [3]. Experimental semivariogram was calculated as

$$\hat{\gamma}(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} [Z(x_i) - Z(x_i + h)]^2 \quad (1)$$

where $N(h)$ denotes the number of data pairs separated by the lag distance h . Fitted variogram was subsequently used to estimate hydraulic conductivity at unsampled locations through OK,

$$\hat{Z}_{\text{OK}}(x_0) = \sum_{i=1}^n \lambda_i Z(x_i), \quad (2)$$

where λ_i are the kriging weights determined from the spatial covariance structure [3]. Within the adopted Maximum Likelihood framework, OK prediction is assumed to provide an estimator of the unknown hydraulic conductivity. Under this assumption, Leave-One-Out Cross-Validation (LOOCV) was performed to evaluate the estimation error associated with the kriging predictions. Residual at each observation was calculated as

$$r(x_i) = Z_{\text{obs}}(x_i) - \hat{Z}_{\text{OK}}^{(-i)}(x_i), \quad (3)$$

where $\hat{Z}_{\text{OK}}^{(-i)}$ denotes the kriging prediction obtained after excluding the corresponding observation. Within this framework, the residuals are interpreted as estimation errors that are not captured by the deterministic geostatistical model. LOOCV residuals were subsequently modelled using RF [2] and GPR [7]. Estimated residual field was then combined with the original OK prediction to generate alternative hydraulic conductivity representations according to

$$\hat{Z}_{\text{corr}}(x) = \hat{Z}_{\text{OK}}(x) + \hat{\delta}(x), \quad (4)$$

where $\hat{\delta}(x)$ denotes machine-learning estimate of the residual field obtained from LOOCV estimation errors.

Resulting hybrid models, referred to as OK-RF and OK-GPR, were evaluated using an independent testing dataset through Root Mean Squared Error (RMSE), coefficient of determination (R^2), and Kling-Gupta Efficiency (KGE). Finally, four hydraulic conductivity representations, namely the homogeneous reference field, deterministic OK field, OK-RF field, and OK-GPR field, were incorporated into the numerical ATES model developed using MRST [5] to investigate their influence on the predicted thermo-hydraulic response under identical operating conditions.

2.2. Numerical ATES Simulations

A three-dimensional coupled groundwater flow and heat transport model was developed using MRST to investigate influence of different hydraulic conductivity representations on the predicted thermo-hydraulic response of an ATES system [5]. System was simulated over a five-year operational period under cyclic seasonal operating conditions.

Four hydraulic conductivity representations were investigated: (i) a homogeneous reference field, (ii) a deterministic OK field, (iii) a hybrid OK-RF field, and (iv) a hybrid OK-GPR field. Each hydraulic conductivity field was converted to intrinsic permeability and implemented within the numerical model. ATES system was simulated over a five-year operational period following a repeated annual cycle of heat injection, thermal recovery, cold injection, and cold recovery.

To ensure a consistent comparison among the investigated scenarios, identical well configurations, operating schedules, boundary conditions, injection temperatures, pumping constraints, thermophysical properties, and numerical settings were maintained throughout all simulations. Consequently, the hydraulic conductivity representation remained the only varying input parameter, and the homogeneous field was adopted as the reference simulation for all subsequent comparisons.

Influence of the different hydraulic conductivity representations was evaluated by comparing thermal plume evolution, production temperatures, well flow rates, bottom-hole pressures (BHP), groundwater flow behaviour, and seasonal heat and cold recovery. Resulting differ-

ences among the simulations were interpreted relative to the homogeneous reference simulation in order to evaluate how alternative hydraulic conductivity representations influence the predicted thermo-hydraulic response of ATES system under identical operating conditions.

3. Case Study

Proposed methodology was applied to Aquifer B, a confined aquifer beneath Parco Sempione, Milan, Italy. Study area covers approximately 1000×1000 m and was selected because hydraulic conductivity measurements obtained from borehole investigations were available for reservoir characterization and subsequent numerical groundwater flow and heat transport simulations.

Hydraulic conductivity dataset consisted of borehole measurements distributed throughout the study area. Available data were randomly divided into 80% training and 20% testing subsets. Training dataset was used to construct OK, OK-RF, and OK-GPR hydraulic conductivity representations, whereas the testing dataset was reserved exclusively for independent model evaluation. Figure 1 illustrates the spatial distribution of the training and testing borehole data used in this study.

Hydrostratigraphic framework of the numerical model was established using the available geological information together with the vertical log K profiles obtained from the borehole data. Principal characteristics of Aquifer B, including the elevations of the upper and lower model boundaries and the modelled aquifer thickness, are summarized in Table 1.

Table 1: Principal characteristics of the modelled Aquifer B.

Parameter	Unit	Value
Surface elevation	m a.s.l.	124.5
Top of Aquifer B	m a.s.l.	83.5
Modelled lower boundary	m a.s.l.	29.5
Modelled thickness	m	54

Figure 2 illustrates the numerical well configuration adopted for ATES simulations. System consists of four hot wells (H1–H4) and nine cold wells (C1–C9) arranged in a modified five-spot well pattern, in which each hot well is surrounded by four neighbouring cold wells and vice versa. Unlike practical ATES instal-

lations, where hot and cold wells are generally positioned as far apart as possible to minimize thermal interference between the hot and cold plumes, this well configuration was intentionally adopted to emphasize the influence of different hydraulic conductivity representations on the predicted thermo-hydraulic response of the numerical model rather than to maximize the thermal efficiency of the ATES system. Throughout all simulations, identical well locations, operating schedules, boundary conditions, pumping conditions, injection temperatures, thermo-physical properties, and numerical settings were maintained. Consequently, the hydraulic conductivity representation remained the only varying input parameter, and the homogeneous hydraulic conductivity field was adopted as the reference simulation for all subsequent comparisons.

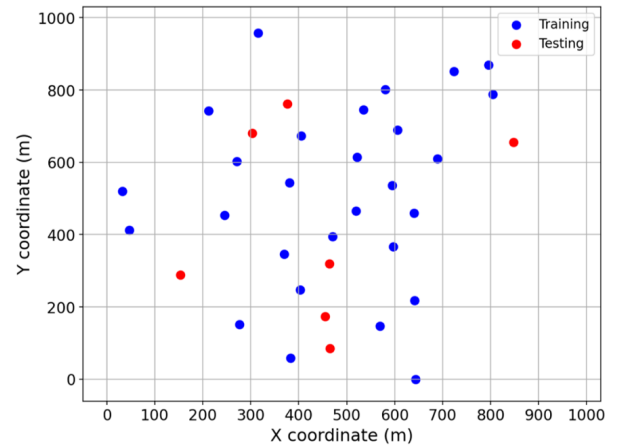


Figure 1: Spatial distribution of the borehole data used for training and testing of the hydraulic conductivity models.

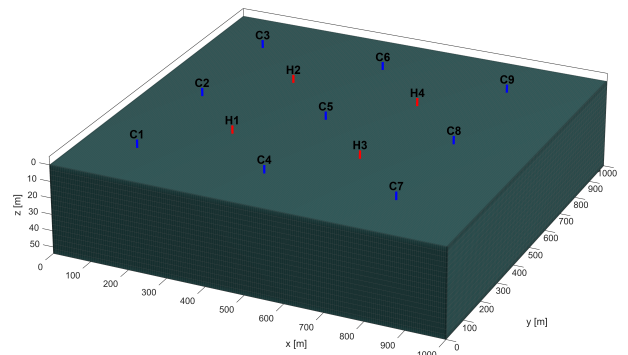


Figure 2: Numerical well configuration adopted for the ATES simulations, showing the modified five-spot well pattern.

4. Results

4.1. Hydraulic Conductivity Characterization

Predictive performance of the OK, OK–RF, and OK–GPR models was evaluated using the independent testing dataset. Figure 3 compares the observed hydraulic conductivity values with the corresponding predictions obtained using the three approaches. OK reproduced the large-scale spatial distribution of hydraulic conductivity, while hybrid OK–RF and OK–GPR models introduced additional local variations through machine-learning-based modelling of the LOOCV estimation errors. Consequently, the three approaches produced different hydraulic conductivity representations while preserving the underlying spatial trends.

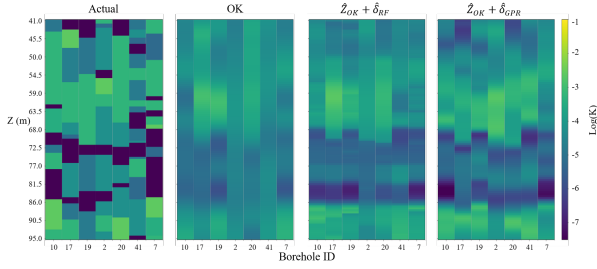


Figure 3: Statistical comparison of the deterministic OK and hybrid hydraulic conductivity representations using the independent testing dataset.

Quantitative evaluation obtained from the independent testing dataset is summarized in Table 2. Relative to the deterministic OK model, both hybrid approaches produced lower RMSE values and higher R^2 and KGE values. The OK–RF model produced the lowest RMSE (1.39) and the highest coefficient of determination ($R^2 = 0.27$), whereas the OK–GPR model produced the highest Kling–Gupta Efficiency (KGE = 0.37). These results indicate that the machine-learning residual models generated alternative hydraulic conductivity representations with different predictive characteristics relative to the deterministic OK model.

Table 2: Statistical comparison of the deterministic OK and hybrid hydraulic conductivity representations using the independent testing dataset.

Dataset	RMSE	R^2	KGE
$\hat{Z}_{OK}$	1.49	0.15	0.15
$\hat{Z}_{OK} + \hat{\delta}_{GP}$	1.44	0.21	0.37
$\hat{Z}_{OK} + \hat{\delta}_{RF}$	1.39	0.27	0.34

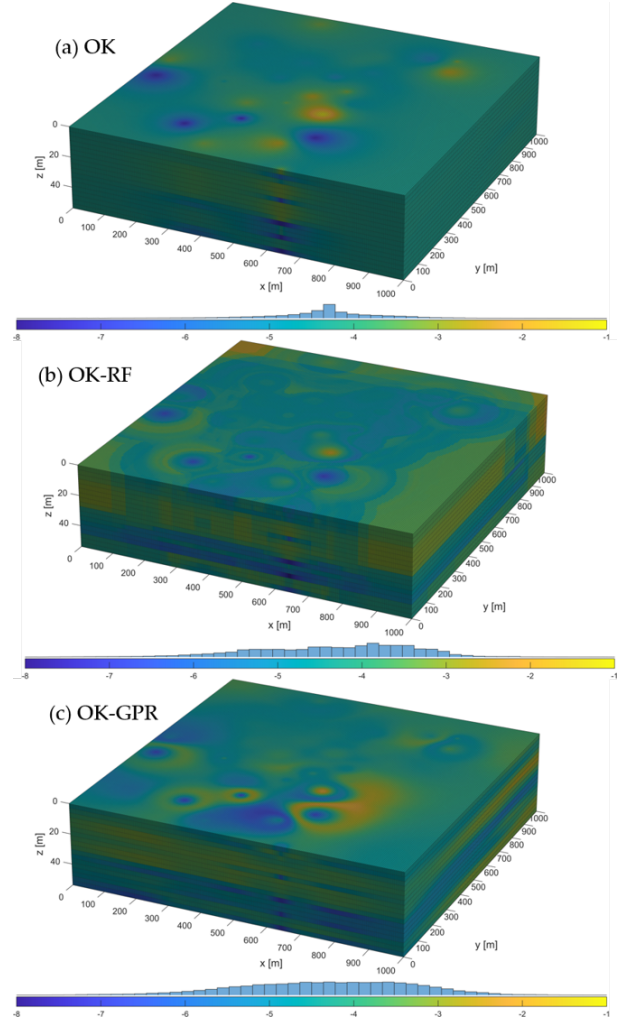


Figure 4: Hydraulic conductivity fields generated using (a) OK, (b) OK–RF, and (c) OK–GPR.

Three hydraulic conductivity representations generated using OK, OK–RF, and OK–GPR are presented in Figure 4. Although all three representations preserve the major spatial patterns inferred from the borehole observations, they exhibit different local spatial characteristics resulting from the adopted characterization approaches. Deterministic OK field exhibits a comparatively smooth hydraulic conductivity

distribution, whereas the OK–RF and OK–GPR fields incorporate additional local spatial variability through machine-learning modelling of LOOCV estimation errors. These alternative hydraulic conductivity representations were subsequently used as input for the numerical ATEs simulations presented in the following section.

4.2. ATEs Performance

Four hydraulic conductivity representations were subsequently incorporated into the three-dimensional numerical ATEs model to investigate their influence on the predicted groundwater flow and heat transport behaviour. Throughout all simulations, identical well configurations, operating schedules, boundary conditions, pumping conditions, thermophysical properties, and numerical settings were maintained. Consequently, the hydraulic conductivity representation remained the only varying input parameter, and the homogeneous hydraulic conductivity field was adopted as the reference simulation. Numerical simulations demonstrate that different hydraulic conductivity representations produce different thermo-hydraulic responses under identical operating conditions. Relative to the homogeneous reference simulation, the heterogeneous hydraulic conductivity fields generated different thermal plume geometries, well temperatures, flow rates, bottom-hole pressures, and seasonal energy recovery. Differences among the simulations became more pronounced during successive operating cycles as seasonal heat injection and extraction continued.

With respect to seasonal energy recovery, the heterogeneous hydraulic conductivity representations generally predicted higher heat recovery than the homogeneous reference simulation. Among the heterogeneous representations, the OK–GPR simulation predicted the highest heat recovery throughout the five-year simulation period. In contrast, the homogeneous reference simulation predicted the highest cold recovery, whereas the heterogeneous representations produced lower cold recovery, with the OK–GPR simulation predicting the lowest values.

Hydraulic responses exhibited larger differences than the thermal responses. Relative to the homogeneous reference simulation, the heterogeneous hydraulic conductivity fields generally predicted larger variations in well flow

rates together with lower bottom-hole pressures, whereas differences in production temperatures were comparatively smaller. Magnitude of these differences varied among the individual wells, indicating that the predicted hydraulic response depends strongly on the local hydraulic conductivity distribution surrounding each well.

Overall, the numerical simulations indicate that the predicted thermo-hydraulic response of the ATEs model is sensitive to the adopted hydraulic conductivity representation. The proposed framework provides a systematic approach for comparing alternative hydraulic conductivity representations and evaluating their influence on the predicted groundwater flow, heat transport, and seasonal thermal energy storage under identical operating conditions.

5. Conclusions

This study developed and evaluated a hybrid geostatistical–machine learning framework for generating alternative hydraulic conductivity representations and investigated their influence on the predicted thermo-hydraulic response of an ATEs system. Within the adopted Maximum Likelihood framework, OK predictions were treated as estimators of the unknown hydraulic conductivity, while cross-validation residuals were interpreted as estimation errors and subsequently modelled using RF and GPR. The resulting hydraulic conductivity representations (OK–RF and OK–GPR) were compared with a homogeneous reference field and a deterministic OK field.

Statistical evaluation demonstrated that the hybrid models produced different predictive characteristics relative to deterministic OK. On the independent testing dataset, the OK–RF model produced the lowest RMSE and the highest coefficient of determination, whereas the OK–GPR model produced the highest KGE. These results indicate that the hybrid approaches generated alternative hydraulic conductivity representations with different statistical characteristics while preserving the underlying spatial trends.

Numerical ATEs simulations demonstrated that the predicted thermo-hydraulic response is sensitive to the adopted hydraulic conductivity representation. Relative to the homogeneous reference simulation, the heterogeneous hydraulic

conductivity fields produced different thermal plume geometries, well temperatures, well flow rates, bottom-hole pressures, and seasonal energy recovery. Among the heterogeneous representations, the OK-GPR simulation predicted the highest heat recovery, whereas the homogeneous reference simulation predicted the highest cold recovery. Simulations also showed that the hydraulic response, represented by well flow rates and bottom-hole pressures, exhibited larger differences among the hydraulic conductivity representations than the corresponding thermal response.

Overall, the proposed framework provides a systematic approach for generating and comparing alternative hydraulic conductivity representations within a consistent numerical modelling framework. Study demonstrates how different representations of hydraulic conductivity influence the predicted groundwater flow, heat transport, and seasonal energy storage behaviour under identical operating conditions, providing a basis for evaluating the sensitivity of numerical ATES simulations to subsurface characterization.

Future research should extend the proposed deterministic framework by incorporating uncertainty quantification through conditional stochastic (Monte Carlo) realizations of hydraulic conductivity. Such an approach would allow uncertainty associated with subsurface characterization to be propagated through groundwater flow and heat transport simulations. Additional work may also investigate alternative machine-learning algorithms, integrate supplementary geological information, and apply the proposed framework to different geological settings and operating ATES systems.

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6. References

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