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Performance of stochastic inversion approaches of groundwater flow and heat transport modeling in parameter estimation

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ABSTRACT

Permeability, thermal conductivity, and porosity distribution are essential determinants of groundwater flow and heat transfer in porous media. The parameter estimation method is extensively employed to comprehend flow and transport dynamics in geothermal systems. With the typically limited resources for conducting field investigations, understanding suitable sampling strategies is crucial before applying a model to site-specific conditions. This study aims to evaluate the performance of stochastic inversion approaches in parameter estimation using Monte Carlo Simulation (MCS) and Ensemble Kalman Filter (EnKF). A synthetic two-dimensional aquifer profile is used to evaluate the accuracy of the estimated hydrothermal properties in accounting for variations in groundwater temperature resulting from cross-hole pumping and injection events. According to the computations of mean absolute and squared errors for estimated hydrothermal properties, the Ensemble Kalman Filter (EnKF) typically yields more precise estimates than Monte Carlo Simulation (MCS). Moreover, the EnKF achieves an equilibrium between precision and efficiency, rendering it the most efficacious method. This study highlights the strengths and limitations of each method, providing valuable insights for selecting appropriate inversion techniques to estimate the parameters in geothermal systems.

Keywords: *stochastic approaches, Monte Carlo Simulation, Ensemble Kalman Filter*

1. Introduction

Permeability, thermal conductivity, and porosity distribution are essential determinants of groundwater flow and heat transfer in porous media. The parameter estimation method is extensively employed to comprehend flow and transport dynamics in geothermal systems. With the typically limited resources for conducting field investigations, understanding suitable sampling strategies is crucial before applying a model to site-specific conditions. This study aims to evaluate the performance of stochastic inversion approaches in parameter estimation using Monte Carlo Simulation (MCS) and Ensemble Kalman Filter (EnKF). A synthetic two-dimensional aquifer profile is used to evaluate the accuracy of the estimated hydrothermal properties in accounting for variations in groundwater temperature resulting from cross-hole pumping and injection events. According to the computations of mean absolute and squared errors for estimated hydrothermal properties, the Ensemble Kalman Filter (EnKF) typically yields more precise estimates than Monte Carlo Simulation (MCS). Moreover, the EnKF achieves an equilibrium between precision and efficiency, rendering it the most efficacious method. This study highlights the strengths and limitations of each method, providing valuable insights for selecting appropriate inversion techniques to estimate the parameters in geothermal systems.

2. Methodologies

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This study concentrates the transient flow and heat transport in vertical, two-dimensional, heterogeneous and saturated aquifer. This section will introduce the methods and ideas used to estimate the governing equations and the assumptions made when simulating flow and heat transport. In previous study, several researchers have published thorough equation derivations and numerical techniques, these will not be mentioned here. Besides, parameters estimation methodologies used in this study to similar with formulas and underlying assumptions used in SHEMAT-suite open.

2.1. Monte Carlo Simulation

This study employs a stochastic modelling sequence utilizing MCS, comprising three primary elements: (1) the generation of a reservoir ensemble via the SGSIM model, (2) the forward modeling of fluid flow and heat transport, and (3) the post-processing restrictions are applied depending on the observed state variables. The fluid flow is described by Darcy's law and the Boussinesq approximation, while heat transport is determined through the application of conservation of energy equations. The model contains the effects of volumetric heat capacity, thermal conductivity, heat production, and the properties of the fluid, such as its density and viscosity. A contraction approach is then used to find the model parameters that best fit the temperature data. State variables are used to find suitable realizations that reflect the different geographical distributions of soil characteristics. These variables come from combined modelling, which integrates random simulations of soil property distributions with the forward model.

2.2. Ensemble Kalman Filter

The EnKF is a stochastic method akin to a large-scale Monte Carlo approach, employing the forward propagation of ensemble members. Data from several boreholes, each with different types of measurements, are combined into a data vector at regular time intervals. This vector is then used to update the system variables using a least-squares method. EnKF is derived from the conventional Kalman filter (Kalman, 1960). EnKF characterizes the probability of the system state through an ensemble of integrated state-parameter vectors produced by Stochastic Geostatistical Simulation as a function in GSLIB (Deutsch and Journel, 1998). All members of the ensemble are equally probable representations of the true states and parameters, based on the available prior knowledge, which includes data and associated uncertainties. This method involves two main steps: a prediction phase, which updates the model state using the forward groundwater flow and heat transport modeling, followed by an analysis phase that revises the ensemble members utilizing observations through the Kalman gain matrix. The state and parameter vector comprises model variables, including hydraulic head (h) and temperature (T), alongside model parameters (permeability (k), porosity (Φ), thermal conductivity (λ)).

3. Illustrative examples

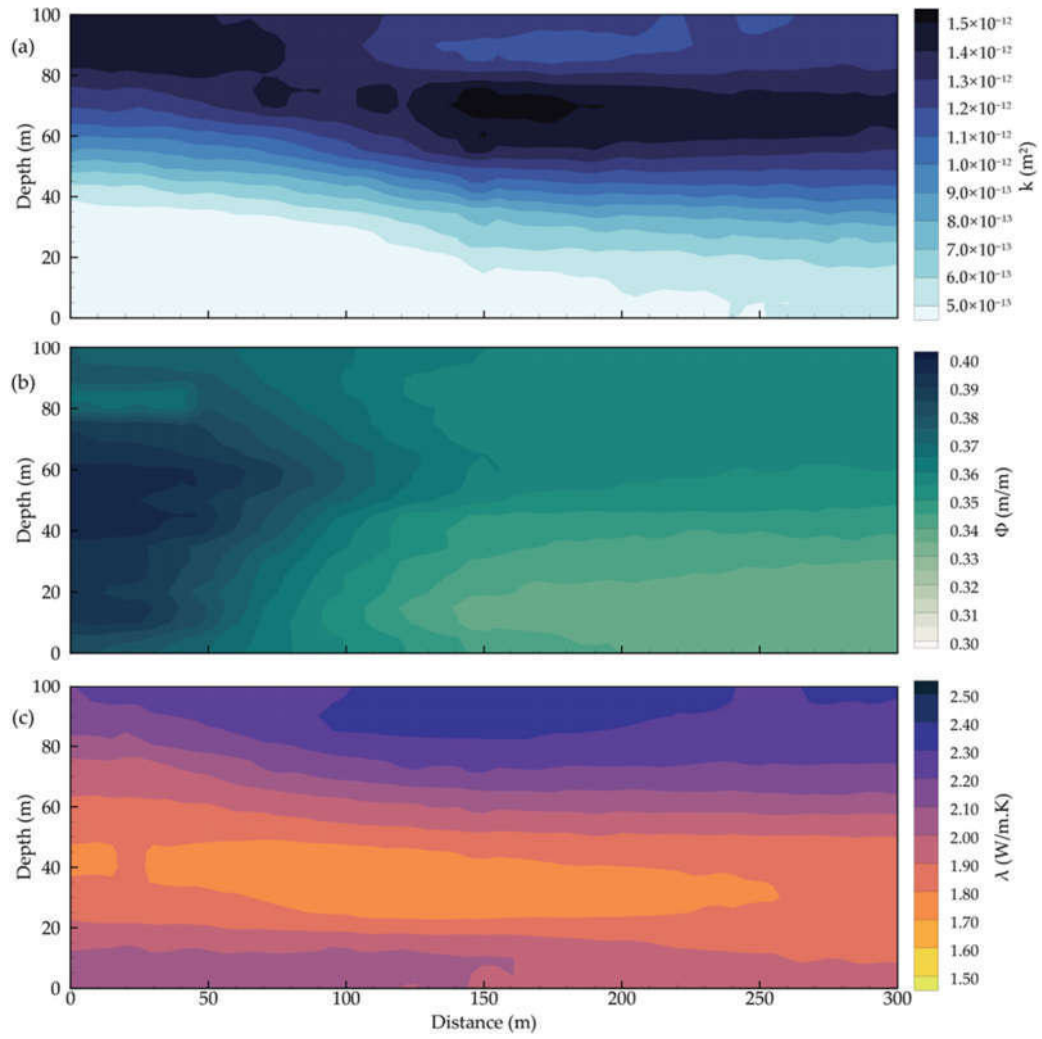


Figure 1. A two-dimensional synthetic aquifer case (a) permeability, (b) porosity, (c) thermal conductivity.

The geometry of the synthetic 2D heterogeneous reservoir has the dimensions 100m by 300m, and is discretized into 1200 elements. Each element has a uniform size of 5m by 5m. The hydraulic and thermal parameters used for the transient case are described in Thuy et al. (2026). Additionally, the conceptual model, boundary and initial conditions are also provided (Thuy et al., 2026). To generate the synthetic measurements, we employed the finite difference scheme to obtain a transient flow and heat transport. Heat is injected into one of the injection wells at a constant rate of $0.001 \text{ m}^3/\text{s}$ and a temperature of 30°C for the injected water. There is also a pumping well with a constant pumping rate of $0.001 \text{ m}^3/\text{s}$. The total simulation time is 1000 days with an interval of 0.1 days. The temperature responses at all 18 observation locations are collected at 0.1, 0.2, 0.3, 0.4, 0.5, 1.0, 1.5, 2.0, 3.0, 5.0, 100, 200, 300, 400, 500, 600, 700, 800, 900, and 1000 days. A total of 18 temperature observations is created later for our inverse model to estimate permeability, thermal conductivity and porosity distributions in the modeling area.

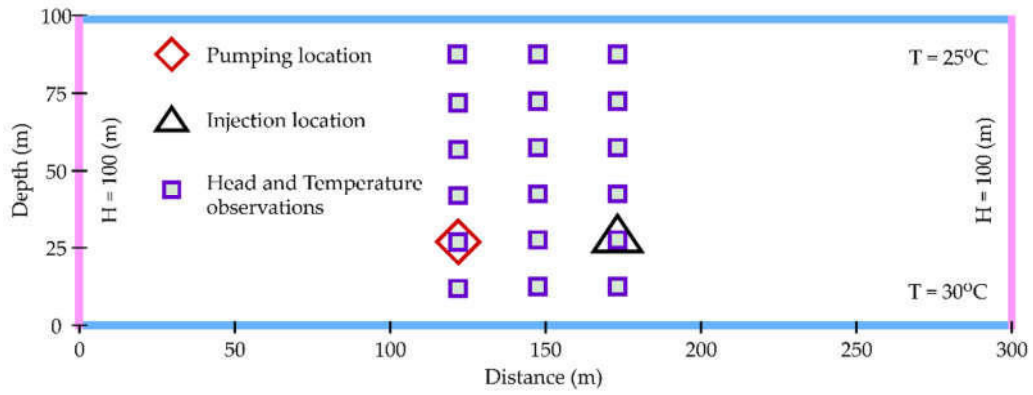


Figure 2. A two-dimensional synthetic aquifer modeling.

4. Results and discussion

4.1. Parameters estimations

Figure 3 compares the estimated and reference values of permeability, porosity, and thermal conductivity (log scale) using Monte Carlo Simulation (MCS; Figures 3a, 3c, 3e) and Ensemble Kalman Filter (EnKF; Figures 3b, 3d, 3e) with 1000 realizations/ensemble members. Overall, both methods show good agreement with the reference data. Permeability exhibits the highest accuracy, with a correlation coefficient of 0.95 for both methods, and low MAE/MSE values, confirming reliable reconstruction. For porosity, the correlation is moderate (0.671), but EnKF outperforms MCS with lower errors, indicating more effective use of observational data during updating. Thermal conductivity also shows strong correlations (0.913 - 0.926), although both methods slightly underestimate low values and overestimate high values.

4.2. Optimization of the number of realizations in the quantification of uncertainties

Figure 4 illustrates the impact of sample size (from 100 to 2000 realizations) on the performance of the stochastic inversion using MCS and EnKF for permeability, porosity, and thermal conductivity. The subplots present evaluation metrics, including correlation coefficient, MAE, and MSE, for each parameter. As the number of samples increases, the correlation coefficients initially improve, indicating better agreement between estimated and reference values. However, beyond approximately 1000 samples (Figures 4a, 4d, and 4g), the correlation coefficients begin to slightly decrease or stabilize, suggesting diminishing returns in accuracy. Similarly, the MAE and MSE values decrease significantly at lower sample sizes but tend to level off and remain nearly constant after 1000 samples across most subplots. This behavior indicates that the models reach a convergence state, where additional realizations do not significantly enhance prediction performance. Overall, Figure 4 demonstrates that both MCS and EnKF achieve stable and reliable results at around 1000 samples, highlighting an optimal balance between computational cost and model accuracy.

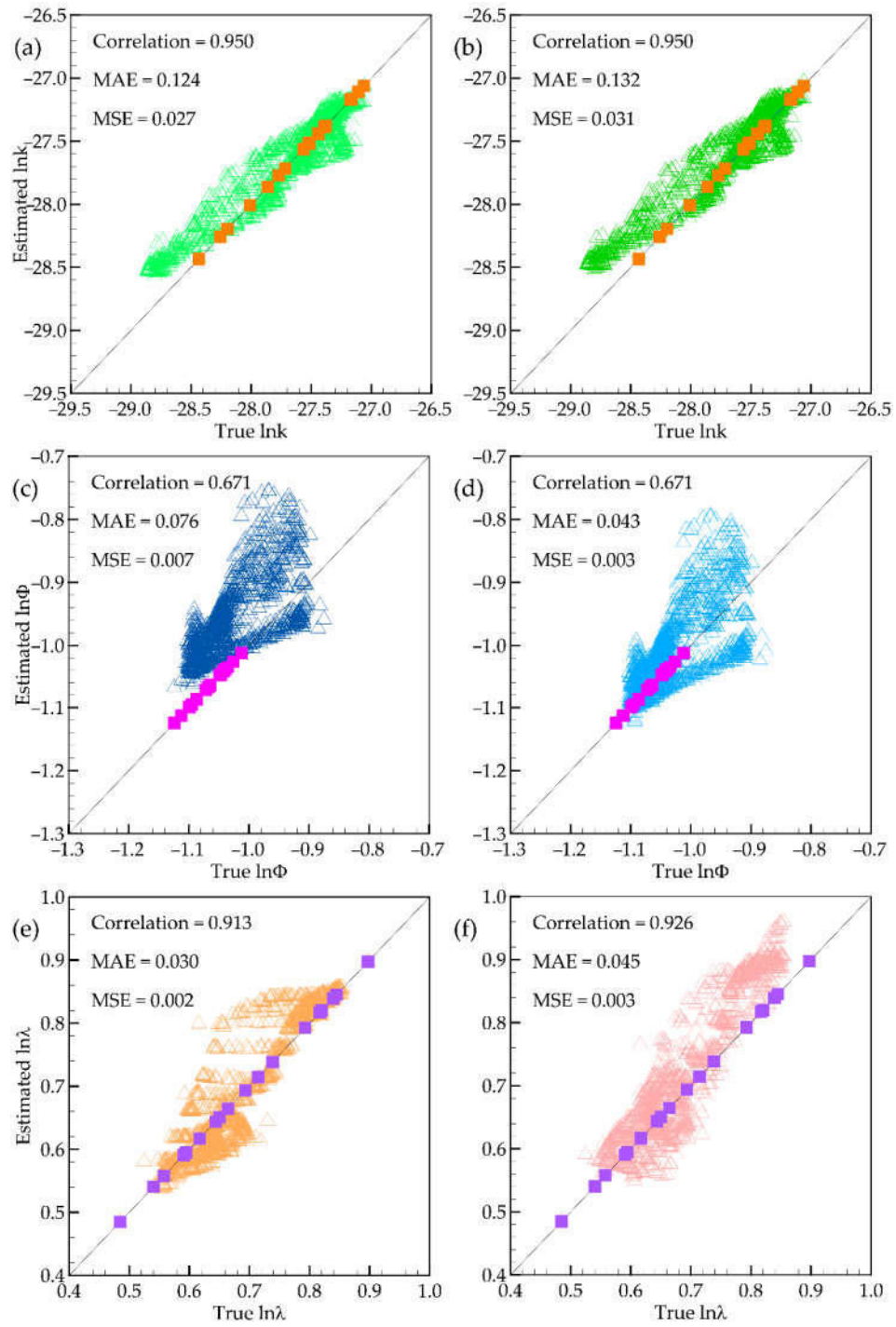


Figure 3. Comparison of parameters estimation using MCS (left column) and EnKF (right column) including permeability (a, b), porosity (c, d), and thermal conductivity (e, f).

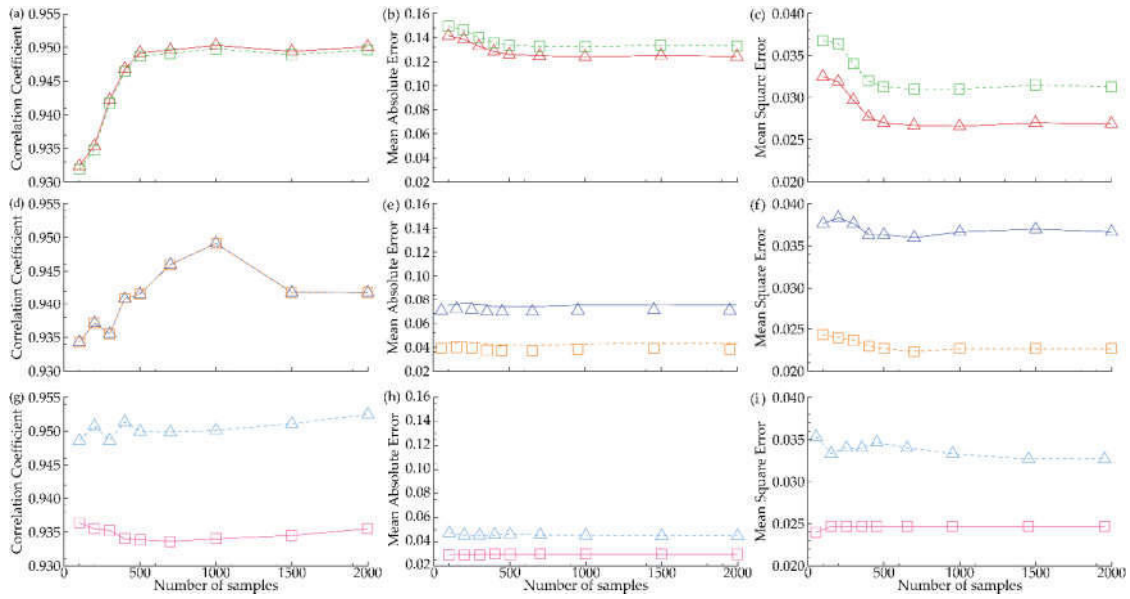


Figure 4. The simulation performance evaluation indicators of parameter estimation including (a - c) permeability, (d - f) porosity, and (g - i) thermal conductivity in natural logarithm scale (top, middle, and bottom, respectively) with correlation coefficient (left), MAE (center), and MSE (right) using MCS (dash line) and EnKF (solid line).

4.3. Cost-effectiveness of in computational cost based on the number of realizations

The existing literature reveals a scarcity of studies demonstrating the efficacy of the EnKF relative to MCS for parameter estimation, especially regarding computational time. A comparative analysis of the computational efficiency and time requirements of the MCS and EnKF, utilizing varying sample sizes (100–2000 realizations for MCS and EnKF, respectively), is illustrated in **Figure 5**. The comparison was conducted using models executed on the identical computer system and hardware. The computational time demands indicate that MCS demonstrates exponential growth, with execution time significantly escalating beyond 500 realizations. Conversely, EnKF exhibits linear scaling, with modest increases in computational time across the entire evaluated range. The findings demonstrate that EnKF retains a computational advantage exceeding sixfold at reduced ensemble sizes (specifically at 100 realizations for MCS), exhibiting consistent superiority across the parameter space, notwithstanding diminishing efficiency ratios up to 2000 ensemble sizes. Despite a slight reduction in the relative advantage of EnKF with increasing ensemble size, it consistently surpasses MCS in all evaluated scenarios. The results indicate that EnKF is a cost-efficient method for managing extensive uncertainty and data integration, especially when simulations are computationally intensive.

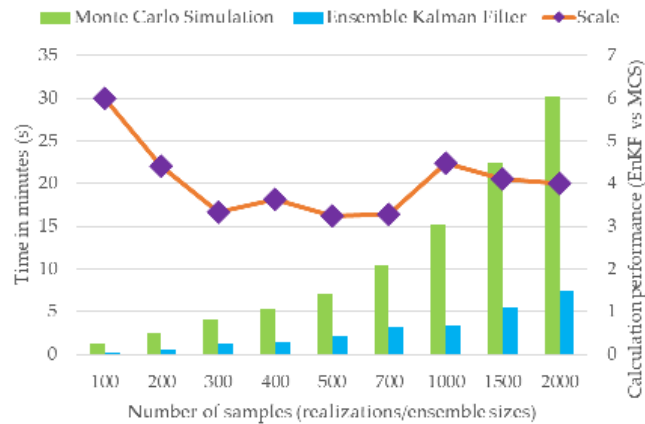


Figure 5. The computational efficiency of MCS and EnKF during the variation of the number of samples.

5. Conclusion

This study quantified the uncertainties associated with hydro-thermal property estimation during cross-hole pumping and injection using stochastic inversion approaches. Both Monte Carlo Simulation (MCS) and Ensemble Kalman Filter (EnKF) successfully reconstructed permeability, porosity, and thermal conductivity with strong agreement to reference values. The results show that uncertainty can be reliably characterized when a sufficient number of samples is used, with convergence achieved at approximately 1000 realizations. In terms of performance, both methods provide comparable accuracy; however, EnKF demonstrates superior computational efficiency and generally lower error metrics due to its data assimilation capability. MCS remains robust but requires a larger number of simulations, leading to higher computational cost. These findings confirm the effectiveness of stochastic inversion methods for hydro-thermal parameter estimation under uncertainty and provide guidance for method selection, with EnKF being more suitable for large-scale or data-driven applications. Applications of this study include geothermal reservoir characterization, optimization of ground-source heat pump systems, and subsurface energy storage. The proposed approach can also be adapted for groundwater management, carbon sequestration, and other subsurface engineering problems where uncertainty quantification is critical.

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