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Evaluation of Parameter Uncertainty Reduction in Groundwater Flow Modeling Using Multiple Environmental Tracers

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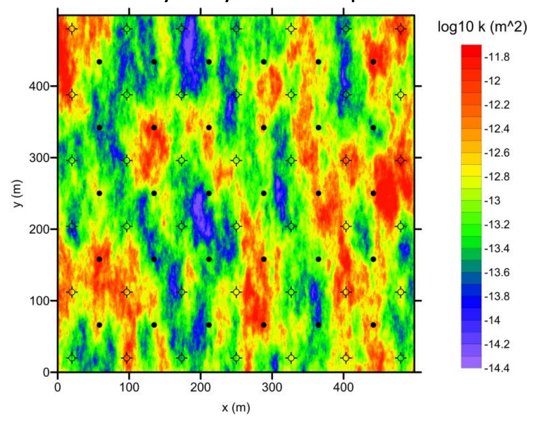
Introduction

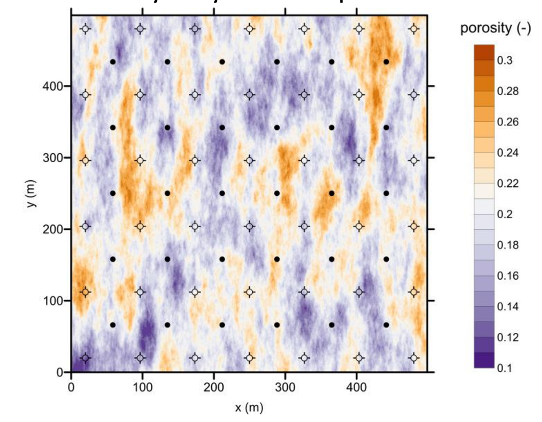
Groundwater environmental tracers can provide important constraints for the calibration of groundwater flow models and significantly reduce the uncertainty in associated model parameters. Direct simulation of environmental tracer concentrations in high-resolution flow and transport models has the additional advantage of avoiding assumptions associated with using calculated groundwater age as a calibration target. The objective of this study is to quantify the reduction in model uncertainty resulting from the addition of environmental tracer concentration data, for individual and combinations of tracers.

The evaluation of uncertainty in groundwater flow model parameters consists of the following steps: (1) development of the conceptual model and construction of a synthetic aquifer, (2) high-resolution simulation of groundwater flow and environmental tracer transport, (3) extraction of synthetic observational data from the simulation results, and (4) automated calibration of a simplified flow and transport model using the pilot point method and the synthetic observational data as calibration targets.

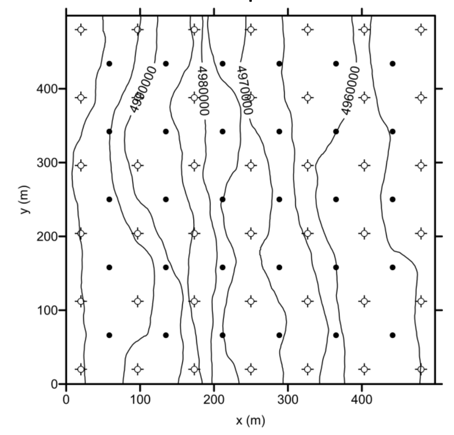
Flow and Tracer Transport Model

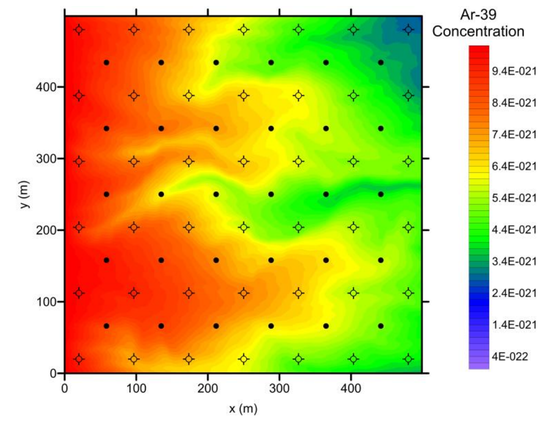
The conceptual model of the groundwater flow system represented in this model is a heterogeneous, anisotropic, confined aquifer consisting of a porous medium with steady-state groundwater flow. Geostatistical simulation is used to create the heterogeneous permeability and porosity fields in the synthetic aquifer of the groundwater model.

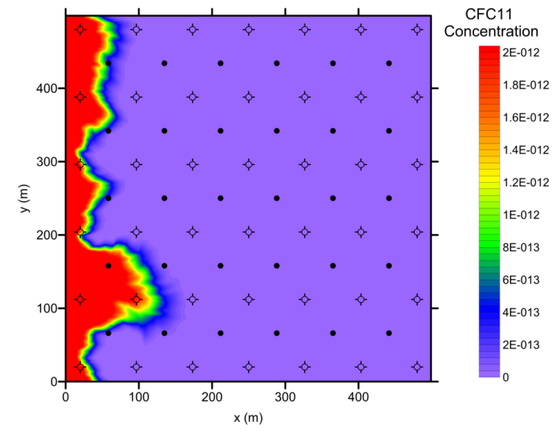


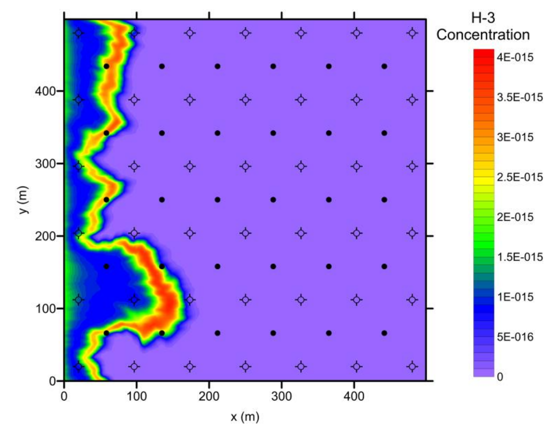


Environmental tracer concentrations are specified in the recharge at the western boundary of the model, based on historical records of atmospheric concentrations. Pre-modern initial conditions for ^{3}H, ^{3}He, and ^{39}Ar are at steady state in the flow system. The groundwater flow and transport model for the synthetic flow system is implemented with the PFLOTRAN software code (Hammond et al. 2012).









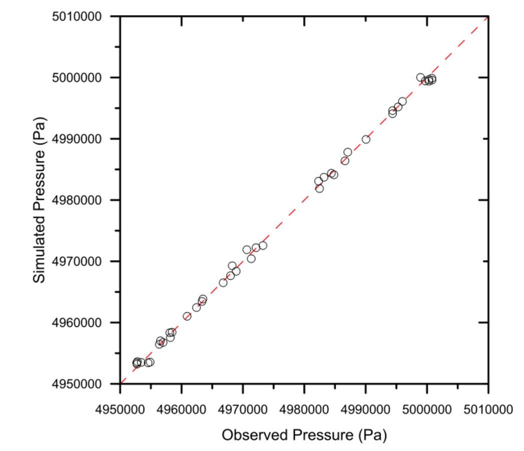
Open crossed circle symbols are observation points and filled circles are pilot points.

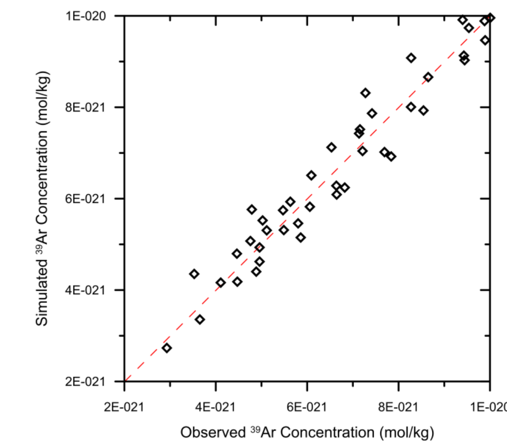
Model Calibration and Parameter Estimation

The simplified groundwater flow and transport model embodies the same conceptual model of the groundwater system described for the synthetic groundwater model, but lacking the detailed knowledge of aquifer heterogeneity in permeability and porosity. The simplified groundwater model represents the kind of model that would be constructed by an investigator who has general knowledge of the geology, dimensions, and boundary conditions of the groundwater system, but data on aquifer properties, pressure, and environmental tracer concentrations at a limited number of observation wells.

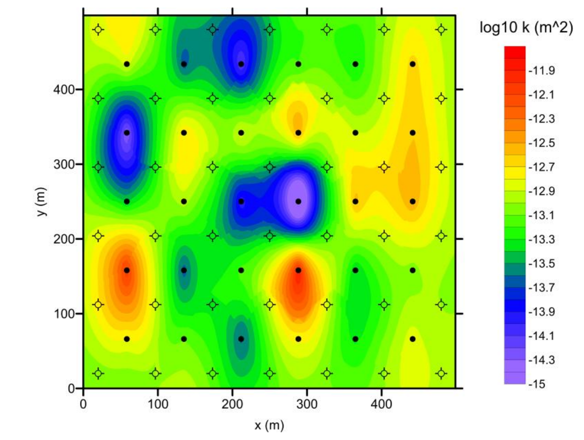
The simplified groundwater flow and transport model is calibrated using automated methods with the PEST software code (Doherty 2009). The pilot point method is often used for the parameterization of heterogeneous fields in groundwater flow model calibration. In this approach, parameter values are assigned at pilot point locations and values are interpolated at other locations based on a measured or assumed spatial correlation structure (de Marsily et al. 1984). The values of permeability at the pilot points are adjusted in the calibration process to obtain an optimal match between observed and simulated pressure and tracer concentrations. Calibration of the simplified groundwater flow and transport model is achieved by minimizing the objective function that is defined by the sum of weighted, squared differences between observed and simulated values of pressure and tracer concentrations. Weighting values for different types of observations (i.e., pressures and different tracer concentrations) are assigned to approximately equalize the contributions of the different observation types to the objective function, thereby assuring equal utilization of information from different data sources. Input parameter values for permeability are log transformed in the calibration process.

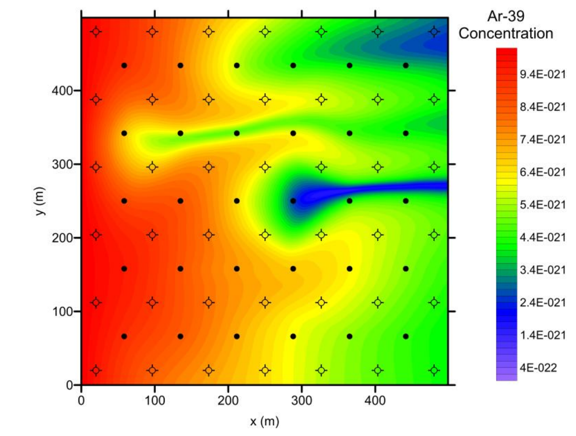
The match between observed synthetic measurements and simulated values using pressure data and ^{39}Ar concentrations is shown graphically in plots of simulated versus observed values below.





Four cases are analyzed by calibration of the simplified groundwater flow and transport model using various combinations of observational data with the PEST code: (1) pressure data only, (2) pressure and CFC11 concentrations, (3) pressure and ^{39}Ar concentrations, and (4) pressure, CFC11, ^{39}Ar, ^{3}H, and ^{3}He concentrations. The automated calibration process successfully achieves minimization of the objective function for all four cases using reasonable ranges of values for permeability at the 30 pilot points. The plot of simulated versus observed ^{39}Ar concentrations above shows a poorer match than for the pressure data, in relative terms. This difference in the calibration results for pressure and ^{39}Ar concentrations is consistent with the fact that fluid pressure is a much more diffusive property of the system than solute concentration.

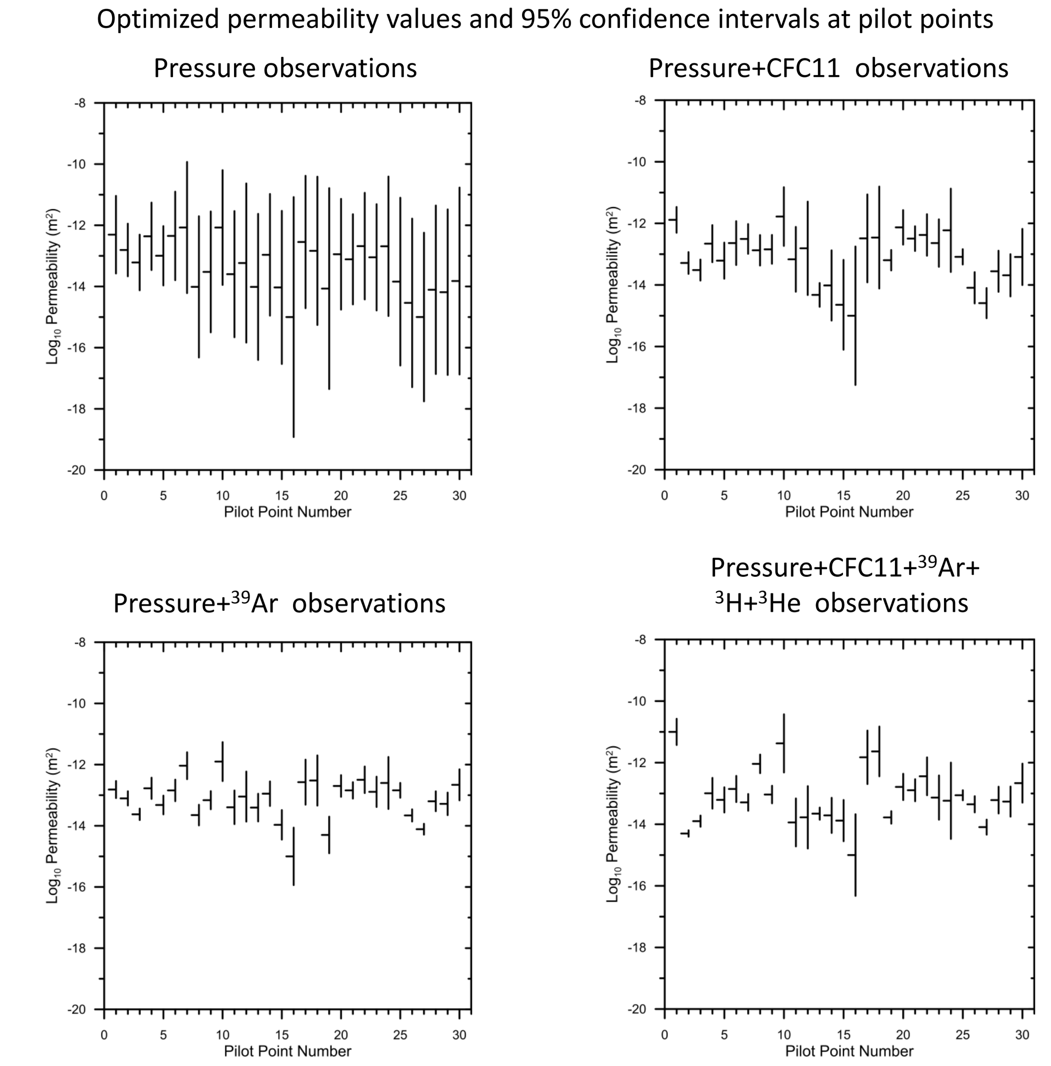




Parameter Uncertainty

Uncertainty in the estimated values of permeability at the 30 pilot points from the calibrated simplified groundwater flow and transport model is evaluated using the linear 95% confidence intervals from the PEST code. Linear uncertainty is calculated from the parameter sensitivities in the Jacobian matrix in the solution space near the optimized model parameters assuming a Gaussian error distribution.

Results indicate a significant reduction in the uncertainty of permeability values at the pilot points with the addition of environmental tracer data, relative to the use of hydraulic measurements alone. Anthropogenic tracers and their decay products such as CFC11, ^{3}H, and ^{3}He provide significant constraint on input permeability values in the model, even when they have not been transported through much of the model domain. Tracer data for ^{39}Ar provide more complete information on aquifer heterogeneity and variability in the flow system, resulting in greater parameter uncertainty reduction.



Case	Observation Data	Average Linear 95% Confidence Interval Width - Log_{10} Permeability (m^2)	Linear Uncertainty Reduction Factor Relative to Case 1
1	pressure	4.6	1.0
2	pressure, CFC11 concentration	1.6	2.9
3	pressure, ^{39}Ar concentration	0.9	5.1
4	pressure,CFC11, ^{39}Ar, ^{3}H, ^{3}He concentrations	1.0	4.6

Conclusions

The direct use of environmental tracer data in groundwater model calibration results in a significant reduction in uncertainty in input parameter estimates for permeability relative to calibration based on hydraulic measurements alone. Tracer data for ^{39}Ar provide even more complete information on the heterogeneity of permeability and variability in the flow system than the anthropogenic tracers, leading to greater uncertainty reduction. Overall, this study demonstrates the effectiveness of directly simulating environmental tracer concentrations in a high-resolution groundwater flow and transport model in the calibration process. With this approach the model directly matches the collected data, effectively bypassing potentially questionable assumptions associated with the calculation of groundwater age from tracer concentrations.

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