

GEOSTATISTICAL INVERSE MODELING: CONSTRAINING ESTIMATION USING SPATIAL AND TEMPORAL AUTOCORRELATION

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INTRODUCTION

Geostatistical inverse modeling is a Bayesian approach that makes use of spatial and/or temporal autocorrelation to regularize the solution of inverse problems. Methods based on this approach can be used to (i) obtain estimates without relying on quantitative prior estimates of the state, (ii) assess and incorporate the influence of auxiliary data, and (iii) objectively estimate the optimal degree of regularization based on available data. Through ongoing work, geostatistical inverse modeling tools are being applied to a variety of problems in environmental engineering and science, such as contaminant source identification in groundwater systems (e.g. Michalak and Kitanidis 2003, 2004) and surface flux estimation of atmospheric trace gases (e.g. Michalak et al. 2004). These tools also show promise for application in other fields where the state parameters exhibits autocorrelation.

BACKGROUND

When a compound is introduced into the environment, whether it be a contaminant released into a groundwater aquifer or a greenhouse gas emitted into the atmosphere, there is often a question as to how and where the compound was released. In the case of groundwater contamination, for example, identifying the source of a pollutant can help in the remediation process and can be critical to the identification of responsible parties. In the case of greenhouse gas emissions, accurate surface flux estimates are needed if we are to design effective emissions control policies. Although these examples appear very different, they both involve the estimation of a spatially and/or temporally autocorrelated state space (e.g. the sources and sinks of a compound) based on measurements of a related variable (e.g. concentrations at monitoring locations) after the compound has been transported and mixed in the environment. Geostatistical inverse modeling methods are increasingly being applied in an effort to solve such problems.

SAMPLE APPLICATION

A sample application illustrating an application to groundwater contaminant source identification is presented in Figures 1 to 3. The data presented in these figures are from the Dover Air Force Base in Delaware, where an unconfined sand aquifer is underlain by a two-layer aquitard (Figure 1). Tetrachloroethene (PCE) and trichloroethene (TCE) are two principal chemical contaminants of the overlying aquifer plume, and concentration profiles for these chemicals have been obtained in the underlying aquitard at several locations. A sample profile for TCE is presented in Figure 2. Note that the sharp jump in the concentration data in the aquitard is associated with strong sorption in the lower aquitard layer and is not necessarily indicative of a pattern in the contamination history. A geostatistical inverse modeling method was applied in an effort to infer the TCE contamination history in the overlying aquifer (Michalak and Kitanidis 2003). The results are presented in Figure 3, along with previous results obtained by Liu and Ball (1999). No prior assumptions were made about the contamination history, and its temporal autocorrelation was inferred from the spatial distribution of the contaminant in the aquitard. In this case, the geostatistical analysis implies that the second concentration peak obtained by Liu and Ball (1999) in the late 1970s may not be an essential feature given the available data.

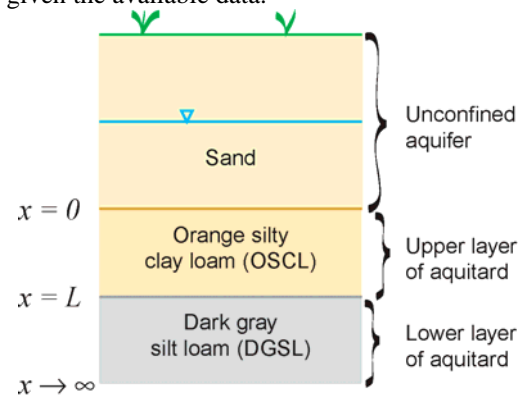


Figure 1. Aquifer/aquitard system at Dover Air Force Base

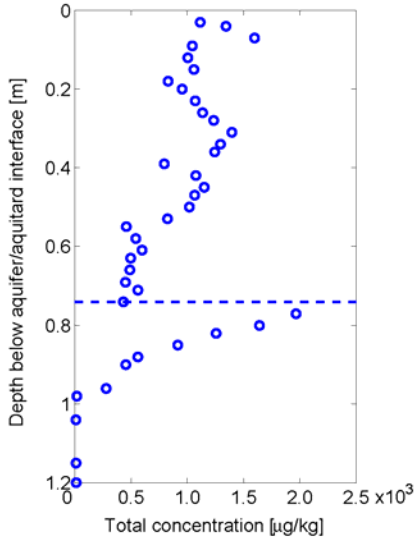


Figure 2. Vertical trichloroethene concentration profile in two-layer aquitard. The dashed line represents the boundary between the two layers of the aquitard.

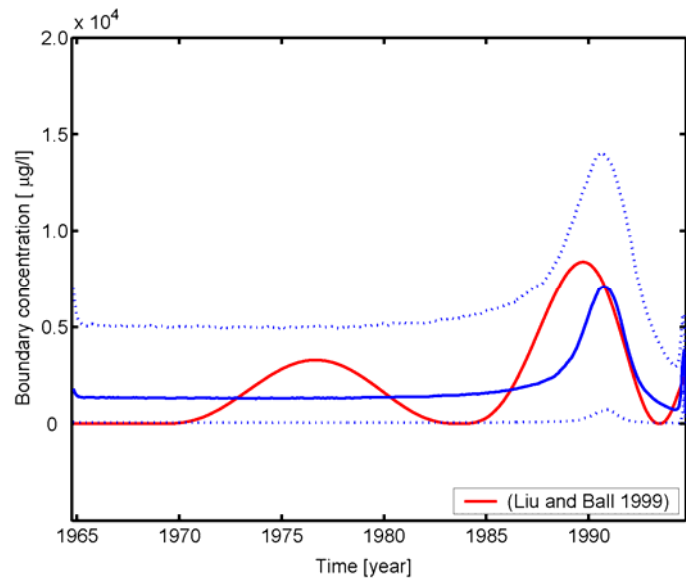


Figure 3. Recovered contamination history in Dover Air Force Base aquifer. The solid blue line represents the best estimate of the contamination history, and the dotted blue lines are the 95% confidence intervals.

REFERENCES

- [1] Liu, C, and W.P. Ball, 1999, "Application of inverse methods to contaminant source identification from aquitard diffusion profiles at Dover AFB, Delaware," *Water Resources Research*, 35(7): 1975-1985.
- [2] Michalak, A.M., and P.K. Kitanidis, 2003, "A Method for Enforcing Parameter Nonnegativity in Bayesian Inverse Problems with an Application to Contaminant Source Identification," *Water Resources Research*, 39(2), 1033, doi:10.1029/2002WR001480.
- [3] Michalak, A.M., and P.K. Kitanidis, 2004, "Estimation of historical groundwater contaminant distribution using the adjoint state method applied to geostatistical inverse modeling," *Water Resources Research*, 40, W08302, doi:10.29/2004WR003214.
- [4] Michalak, A.M., L. Bruhwiler, and P.P. Tans, 2004, "A geostatistical approach to surface flux estimation of atmospheric trace gases," *Journal of Geophysical Research*, 109, D14109, doi:10.1029/2003JD004422.

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