Effects of Temporal Error Correlation on Quantification of Predictive Uncertainty in Groundwater Reactive Transport Modeling

Student Abstract

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Quantifying uncertainty of reactive transport simulations in groundwater can be conducted by using multiple conceptual models because groundwater flow and reactive processes are complex and subject to multiple interpretations. Consideration of alternative models results in broader but more realistic estimates of predictive uncertainty because the alternatives capture different plausible conceptual uncertainties. When quantitatively comparing model simulations it is important to separate error introduced by the inherent random processes in a groundwater aquifer from the structural error introduced by considering an alternative plausible conceptual model. Model structural error is likely to present a high degree of temporal correlation for breakthrough data collected sequentially along time. It has been long recognized that the error correlation may affect parameter estimation and predictive uncertainty quantification. However, methods for accurately describing the correlation structure of the errors and to incorporate it into groundwater reactive transport modeling is an open question. In conventional groundwater modeling, the errors are assumed to be multivariate Gaussian with zero mean and independent with a diagonal covariance matrix by considering only variances of measurement errors. This assumption has been found invalid in reactive transport modeling, and may lead to significant underestimation of predictive uncertainty. This is particularly true in multimodel analysis when alternative reactive transport models are considered. Use of a diagonal covariance matrix of the measurement errors in the calibration can cause one model to have an overwhelmingly high model probability (even 100%), which cannot be justified by the available data and knowledge.

In this study, we developed a statistical method to identify the temporal correlation structure using time series theories. The method considers both measurement errors and model structural errors. Unlike the measurement errors, the model structural errors present a high degree of temporal correlation. Therefore, unlike the conventional assumption, the correlation structure of the total errors is characterized by a full covariance matrix instead of the diagonal one. The full covariance matrix is obtained by simulating the correlated errors with autoregressive models and is incorporated into groundwater modeling by an iterative method with two stages of parameter estimation. We applied this method to a set of synthetic and real-world surface complexation models developed to simulate uranium transport based on a series of column experiments. Our results demonstrated that (1) the errors are highly temporally correlated due to model structural errors; (2) the temporal correlation can be properly considered by our method; (3) if the error correlation is disregarded, model uncertainty is underestimated, and predictive uncertainty bound is narrow, hardly covering the true values; and (4) with the error correlation considered by using our method, the predictive uncertainties of individual models become larger, and the model probabilities become distributed more evenly and realistically among the models, thus leading to better predictive performance with considering model uncertainty. Our method is mathematically general and theoretically can be applied to any reactive transport models. Our future research is to further evaluate and develop the method for multi-scale models and datasets.