Geophysical Research Abstracts
Vol. 15, EGU2013-3712, 2013
EGU General Assembly 2013

Use of Data-driven Models to Enhance Prediction of Groundwater Models

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Physically-based models are powerful quantitative tools to analyze groundwater flow and solute transport. As these models are being used to inform decisions that have enormous social, political and economic impacts upon stake-holders, there are increasing requirements for their accuracy. On the other hand, it is widely recognized that groundwater models are subjected to uncertainty associated with model structure, parameter, input data and measurements used to evaluate the model. Common practice is to use regression-based calibration to estimate model parameters and associated uncertainty from historical data; the calibrated model is then used for prediction. Prediction uncertainty is typically quantified using confidence intervals, which are computed by propagating parameter uncertainty through the model. Nevertheless, the unavoidable uncertainty associated with physically-based groundwater models often results in both aleatoric and epistemic model calibration errors, thus violating a key assumption for regression-based parameter estimation and uncertainty quantification.

We propose a complementary modeling approach to enhance the prediction of calibrated groundwater models. First, we develop data-driven models (DDMs) based on machine learning techniques to account for the epistemic error (bias) of the groundwater model. By learning from historical residuals of a calibrated groundwater model, the DDMs are capable of correcting its bias when the model is used for forecasting or extrapolation purposes. Two machine learning techniques, the instance-based weighting and support vector regression, are used to build the DDMs. Second, we characterize the aleatoric component of predictive uncertainty by fitting a probability distribution to the error remaining after bias correction by DDMs. We then calculate the prediction interval by imposing the aleatoric error distribution on the DDMs-corrected prediction of interest of the physically-based groundwater model. We test the proposed approach on synthetic and real-world case studies. In both cases, the DDMs effectively reduce the predictive bias of the groundwater models. We further evaluate the calculated prediction intervals by comparing the coverage probability with their significance level. Preliminary results show that the proposed approach yields reliable prediction intervals. This computationally efficient approach is especially suitable for cases where the simulation results of existing calibrated groundwater model do not satisfactorily agree with (possibly newly acquired) observations, yet it is not feasible to re-calibrate the model or develop a new model.