Geophysical Research Abstracts Vol. 12, EGU2010-5676-1, 2010 EGU General Assembly 2010 © Author(s) 2010



## "A space-time ensemble Kalman filter for state and parameter estimation of groundwater transport models"

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Herrera (1998) proposed a method for the optimal design of groundwater quality monitoring networks that involves space and time in a combined form. The method was applied later by Herrera et al (2001) and by Herrera and Pinder (2005). To get the estimates of the contaminant concentration being analyzed, this method uses a space-time ensemble Kalman filter, based on a stochastic flow and transport model. When the method is applied, it is important that the characteristics of the stochastic model be congruent with field data, but, in general, it is laborious to manually achieve a good match between them. For this reason, the main objective of this work is to extend the space-time ensemble Kalman filter proposed by Herrera, to estimate the hydraulic conductivity, together with hydraulic head and contaminant concentration, and its application in a synthetic example.

The method has three steps: 1) Given the mean and the semivariogram of the natural logarithm of hydraulic conductivity (ln K), random realizations of this parameter are obtained through two alternatives: Gaussian simulation (SGSim) and Latin Hypercube Sampling method (LHC). 2) The stochastic model is used to produce hydraulic head (h) and contaminant (C) realizations, for each one of the conductivity realizations. With these realization the mean of ln K, h and C are obtained, for h and C, the mean is calculated in space and time, and also the cross covariance matrix h-ln K-C in space and time. The covariance matrix is obtained averaging products of the ln K, h and C realizations on the estimation points and times, and the positions and times with data of the analyzed variables. The estimation points are the positions at which estimates of ln K, h or C are gathered. In an analogous way, the estimation times are those at which estimates of any of the three variables are gathered. 3) Finally the ln K, h and C estimate are obtained using the space-time ensemble Kalman filter. The realization mean for each one of the variables is used as the prior space-time estimate for the Kalman filter, and the space-time cross-covariance matrix of h-ln K-C as the prior estimate-error covariance-matrix.

The synthetic example has a modeling area of 700 x 700 square meters; a triangular mesh model with 702 nodes and 1306 elements is used. A pumping well located in the central part of the study area is considered. For the contaminant transport model, a contaminant source area is present in the western part of the study area. The estimation points for hydraulic conductivity, hydraulic head and contaminant concentrations are located on a submesh of the model mesh (same location for h, ln K and c), composed by 48 nodes spread throughout the study area, with an approximately separation of 90 meters between nodes.

The results analysis was done through the mean error, root mean square error, initial and final estimation maps of h, ln K and C at each time, and the initial and final variance maps of h, ln K and C. To obtain model convergence, 3000 realizations of ln K were required using SGSim, and only 1000 with LHC. The results show that for both alternatives, the Kalman filter estimates for h, ln K and C using h and C data, have errors which magnitudes decrease as data is added.

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