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A coupled stochastic inverse-management framework for dealing with nonpoint agriculture pollution under groundwater parameter uncertainty

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SUMMARY

In this paper a methodology for the stochastic management of groundwater quality problems is presented, which can be used to provide agricultural advisory services. A stochastic algorithm to solve the coupled flow and mass transport inverse problem is combined with a stochastic management approach to develop methods for integrating uncertainty; thus obtaining more reliable policies on groundwater nitrate pollution control from agriculture. The stochastic inverse model allows identifying non-Gaussian parameters and reducing uncertainty in heterogeneous aquifers by constraining stochastic simulations to data. The management model determines the spatial and temporal distribution of fertilizer application rates that maximizes net benefits in agriculture constrained by quality requirements in groundwater at various control sites. The quality constraints can be taken, for instance, by those given by water laws such as the EU Water Framework Directive (WFD). Furthermore, the methodology allows providing the trade-off between higher economic returns and reliability in meeting the environmental standards. Therefore, this new technology can help stakeholders in the decision-making process under an uncertainty environment. The methodology has been successfully applied to a 2D synthetic aquifer, where an uncertainty assessment has been carried out by means of Monte Carlo simulation techniques.

1. Introduction

Groundwater is the ultimate source of freshwater to sustain many important agricultural production areas when surface water sources have been depleted. Furthermore, irrigation is the most important water use accounting for about 70% of the global freshwater withdrawals and 90% of consumptive water uses. Although the development of an intensive agriculture represents one of the main factors in the current economic development of many regions, it has also become an important environmental issue in recent years. This is because it poses many impacts and threats to groundwater bodies, such as overdrafting, aquifer pollution, impacts on downstream demands or impacts on Groundwater Dependent Ecosystems (GDEs). Different water laws and policies around the world deal with such problems. For instance, the EU Water Framework Directive (EC, 2000) stipulates that groundwater bodies must achieve a good chemical and quantitative status by a set deadline.

However, the decision-making process in groundwater management protection is complex because of heterogeneous stakeholder interests, multiple objectives, key drivers influencing the agricultural market and farmer's decisions, land-use/crop pattern evolution and uncertain outcomes. A wide range of stakeholders play an active role in water resources management. They range from irrigation communities, government, river basin authority, Non-Governmental Organisations (NGO's), agri-business industries, farmers to electric power industries (because of groundwater abstraction costs). Moreover, integrated water resources management incorporates technical, scientific, political, legislative and organizational aspects of a water system. Because of that, stakeholders need new technologies and tools to help them in the decision-making process. This links with the main goal of this paper, which is to present a hydro-economic modeling framework for agricultural advisory services. Specifically, this work is intended to analyze the influence of uncertainty in the physical parameters of a heterogeneous groundwater diffuse pollution problem on the results of management strategies, and to introduce methods that integrate uncertainty and reliability in order to obtain strategies of spatial allocation of fertilizer use in agriculture.

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The methodology is based on the coupling of a stochastic inverse model to identify non-Gaussian parameters and to reduce uncertainty in heterogeneous aquifers with a groundwater quality management model for dealing with non-point agriculture pollution. This coupling entails the use of different models (groundwater flow, mass transport, agronomic, economic and optimization models) to assess the effect of uncertainties on the economically optimal decisions. Then, the underlying biophysical processes of pollution formation and pollution transport and fate are explicitly taken into account. It should be mentioned that a small number of papers in the literature have developed a similar approach as that here presented (e.g., Bakr et al., 2003). Furthermore, they were intended to design pump-and-treat groundwater remediation strategies.

The stochastic inverse model allows identifying non-Gaussian parameters and reducing uncertainty in flow and mass transport predictions by constraining stochastic simulations to data, while the optimization management model determines the spatial and temporal distribution of fertilizer application rates that maximizes net benefits in agriculture constrained by quality requirements in groundwater at various control sites.

Inverse modeling has become an important and necessary step in hydrogeological studies (e.g., Poeter and Hill, 1997). This is because the inability to characterize subsurface heterogeneity properly makes predictions of groundwater contamination highly uncertain. Consequently, the predictions of management models based on groundwater quality standards are also uncertain. The literature on groundwater inverse modeling mostly focuses on the estimation of parameters and its underlying uncertainty. This is because they are the most relevant factors affecting mass transport predictions (Smith and Schwartz, 1981) and because conceptual uncertainties are difficult to be formalized in a rigorous mathematical framework (Renard, 2007). Regarding the different groundwater parameters we have focused on the hydraulic conductivity, owing to the fact that it is the paramount parameter controlling the flow and solute transport in groundwater. In fact, it can vary spatially by several orders of magnitude. For instance, the aquifer at the Columbus Air Force Base in Mississippi, commonly known as the Macrodispersion Experiment (MADE) site, is a strongly heterogeneous system with a variance of the natural logarithm of K of nearly 4.5 (e.g., Rehfeldt et al., 1992).

Eventually, once the groundwater parameter uncertainty has been strongly reduced by the inverse model, more reliable policies can be defined using the hydro-economic model. It explicitly integrates nitrate leaching and fate and transport in groundwater with the economic impacts of nitrogen fertilizer restrictions in agriculture.

The remaining of the paper is organized as follows: firstly, a background of the stochastic inverse model and the management model is presented; secondly, the methodology has been verified on a 2D synthetic case. Finally, we have highlighted the advantages of using the methodology for providing agricultural advisory services to policy-makers.

2. Modeling framework

The methodology is based on the coupling of a stochastic inverse model to identify non-Gaussian parameters and to reduce uncertainty in heterogeneous aquifers with a groundwater quality management model for dealing with non-point agriculture pollution. An explanation of both models is provided below:

2.1. Stochastic inverse model (the GC method)

The GC method is a stochastic inverse modeling technique for the simulation of conductivity (K) fields in aquifers which has been developed to overcome several of the limitations found in the already existing techniques (Llopis-Albert, 2008; Capilla and Llopis-Albert, 2009). The method was exhaustively verified on a 2D synthetic aquifer (Llopis-Albert and Capilla, 2009a). In addition, a 3D application to the Macrodispersion Experiment (MADE-2) site, on a highly heterogeneous aquifer at Columbus Air Force Base in Mississippi (USA) was presented by Llopis-Albert and Capilla (2009b); and also on a complex real-world case study in a fractured rock site (Llopis-Albert and Capilla, 2010a). Furthermore, it was extended to deal with independent stochastic structures belonging to independent K statistical populations (SP) of fracture families and the rock matrix, each one with its own statistical properties (Llopis-Albert and Capilla, 2010b).

The method uses an iterative optimization procedure to simulate K fields honoring K measurements, secondary information obtained from expert judgment or geophysical surveys, transient piezometric head (h) data and concentration (c) measurements. Travel time data can also be considered by means of a backward-in-time probabilistic model (Neupauer and Wilson, 1999), which extends the applications of the method to the characterization of sources of groundwater contamination. The formulation of the method does not require assuming the classical multi-Gaussian hypothesis allowing the reproduction of strings of extreme values of K that often take place in nature, being these formation features crucial in order to obtain realistic and safe estimations of mass transport predictions (Gómez-Hernández and Wen, 1998; Zinn and Harvey, 2003; Llopis-Albert and Capilla, 2009b; Zhou et al., 2013). In this sense, the probabilities of very short travel times could be severely underestimated using the multi-Gaussian approach, since it implies the minimal spatial correlation of extreme values. Then the multi-Gaussian approach may not reproduce some geological settings, e.g., channeling that are critical for mass transport. This may lead to travel times ten times slower than those predicted by taking into account the non-Gaussianity feature (Gómez-Hernández and Wen, 1998).

The method has been developed using a modified version of the gradual deformation technique (Hu, 2000), and applying a Lagrangian approach to solve the mass transport equation. This allows avoiding numerical dispersion usually found in Eulerian approaches. The algorithm has been implemented for 3D transient flow problems under variable density flow conditions, considering the dispersion as a tensorial magnitude, and a first-order mass transfer approach. Performing a Bernoulli trial on the appropriate phase transition probabilities, the particle distribution between the mobile domain and the immobile domain can be determined (Salamon et al., 2006).

The iterative optimization process for constraining stochastic simulations to data is carried out by doing non-linear combinations of seed conditional realizations. These seed conductivity (K) fields are already conditional to K and secondary data, and are generated by sequential indicator simulation. The a priori stochastic structure of these K seed fields is defined by means of the local conditional cumulative density functions (ccdf's) and the indicator variograms, thus allowing the GC method to adopt any Random Function (RF) model. As a first step, the GC method builds linear sequential combinations of non multiGaussian K fields that honor K data:

$$K^m = \alpha_1 K^{m-1} + \alpha_2 K_{2m} + \alpha_3 K_{2m+1} \quad \text{with } K_0 = K^1 \tag{1}$$

where subscripts stand for seed fields and superscripts for conditional fields resulting from a previous linear combination That is, at m iteration, the field K^{m-1}, from the previous iteration, is combined with two new independent realizations K_{2m} and K_{2m+1}. The procedure requires combining at least three conditional realizations at a time to ensure the preservation of mean, variance, variogram