Journal of Hydrology 533 (2016) 180–190

Contents lists available at ScienceDirect

Journal of Hydrology

journal homepage: www.elsevier.com/locate/jhydrol

Pareto-based efficient stochastic simulation–optimization for robust and reliable groundwater management

J. Sreekanth [a,*], Catherine Moore [b,c], Leif Wolf [d]

[a] Commonwealth Science and Industrial Research Organisation, Land and Water Flagship, Dutton Park, Australia
[b] Environmental Science and Research, New Zealand
[c] GNS Science, New Zealand
[d] Karlsruhe Institute of Technology, Germany

ARTICLE INFO

Article history:
Received 1 April 2015
Received in revised form 30 September 2015
Accepted 1 December 2015
Available online 14 December 2015
This manuscript was handled by Andras Bardossy, Editor-in-Chief, with the assistance of Wolfgang Nowak, Associate Editor

Keywords:
Simulation–optimization
Groundwater management
Uncertainty quantification
Monte Carlo analysis
Decision making under uncertainty

SUMMARY

Simulation–optimization methods are used to develop optimal solutions for a variety of groundwater management problems. The true optimality of these solutions is often dependent on the reliability of the simulation model. Therefore, where model predictions are uncertain due to parameter uncertainty, this should be accounted for within the optimization formulation to ensure that solutions are robust and reliable. In this study, we present a stochastic multi-objective formulation of the otherwise single objective groundwater optimization problem by considering minimization of prediction uncertainty as an additional objective. The proposed method is illustrated by applying to an injection bore field design problem. The primary objective of optimization is maximization of the total volume of water injected into a confined aquifer, subject to the constraints that the resulting increases in hydraulic head in a set of control bores are below specified target levels. Both bore locations and injection rates were considered as optimization variables. Prediction uncertainty is estimated using stacks of uncertain parameters and is explicitly minimized to produce robust and reliable solutions. Reliability analysis using post-optimization Monte Carlo analysis proved that while a stochastic single objective optimization failed to provide reliable solutions with a stack size of 50, the proposed method resulted in many robust solutions with high reliability close to 1.0. Results of the comparison indicate potential gains in efficiency of the stochastic multi-objective formulation to identify robust and reliable groundwater management strategies.

1. Introduction

Coupled simulation–optimization methods are used to identify optimal groundwater management solutions for a variety of problems, such as the identification and remediation of groundwater pollutant sources, or the identification of optimal and sustainable management rules for coastal aquifers or wetlands (Gorelick, 1983; Gorelick et al., 1984; Ahlfeld and Pinder, 1992; Feyen and Gorelick, 2004; Ayvaz and Karahan, 2008; Sreekanth and Datta, 2010, 2011a,b). The groundwater flow and transport models used in these simulation–optimization methods are typically populated with uncertain parameter estimates, in particular heterogeneous hydraulic conductivity parameter fields. Even when large amount of groundwater monitoring data is available for constraining the model, unique estimation of the spatially varying parameters may be difficult. Many realizations of parameters can often be estimated which reproduces the calibration data (Tonkin and Doherty, 2009). The parameter uncertainty is propagated through the model simulation process, resulting in prediction uncertainty. The optimal solution identified by considering one set of model parameters in the coupled simulation–optimization may become sub-optimal or even infeasible when other combination of plausible parameters are considered in the model, questioning the reliability of the optimal solution. This paper presents a novel and efficient method for accounting for this uncertainty within the simulation–optimization to provide reliable and robust solutions. In this context, robust solutions can be defined as solutions which are less sensitive to perturbations in the parameters defining the objective function and system constraints (Deb and Gupta, 2006); reliability is defined in terms of the probability of satisfying the constraints (Feyen and Gorelick, 2004).

Early methods to evaluate the effect of model parameter uncertainty on optimal groundwater management solutions were

* Corresponding author at: Commonwealth Science and Industrial Research Organisation, Land and Water Flagship, 41 Boggo Road, Dutton Park, Queensland 4012, Australia.

E-mail address: Sreekanth.janardhanan@csiro.au (J. Sreekanth).

http://dx.doi.org/10.1016/j.jhydrol.2015.12.001
0022-1694/© 2015 Elsevier B.V. All rights reserved.

initially reviewed in Gorelick (1983). One earliest approach is called the 'chance-constrained optimization method. In this method probability density function of the uncertain parameter is evaluated and the model predictions corresponding to a certain percentile of this distribution are included in the optimization formulation as constraints. Thus, in spite of considering the entire distribution of uncertain parameters only a single parameter realization corresponding to a certain percentile is incorporated in the optimization formulation. However, when considering uncertain parameters, the optimal solution is typically not dictated by one single worst case realization. Instead part of one realization dictates the optimal solution in one region, and parts of another realization dictate the optimal solution in another region. Therefore a reliable optimal solution usually cannot be found from a single realization (Feyen and Gorelick, 2004).

To address the absence of any single worst case realization, more recent simulation–optimization efforts consider multiple parameter realizations, and their corresponding aquifer response, in a 'stochastic optimization' procedure. In this framework each candidate "optimal" solution to the groundwater optimization problem is tested with multiple model runs, each with a distinct realization of the uncertain parameter field. The modeled aquifer response, for example – the resulting hydraulic head at observation locations, is tested for violation of constraints imposed by the optimization formulation. Multiple realization (or stochastic) optimization uses a "stacking approach", where a small number of realizations are selected and an optimal solution is obtained which is reliable for all of the realizations in the stack (Feyen and Gorelick, 2004; Bayer et al., 2008, 2010). A number of such stochastic optimization formulations for developing optimal groundwater management solutions have been reported (Wagner and Gorelick, 1987, 1989; Morgan et al., 1993; Datta and Dhiman, 1996; Smalley et al., 2000; Zheng and Wang, 2002; Ricciardi et al., 2007; Sreekanth and Datta, 2011a,b, 2013). In some studies using this approach, reliability of the optimal solutions is tested outside the optimization framework using Monte Carlo analyses with a much larger number of realizations (Chan, 1993; Feyen and Gorelick, 2004). However the post optimization reliability testing, which uses a larger number of realizations than the stack size, often reveals that many realizations fail to meet optimization constraints. Feyen and Gorelick (2004) proposed a formula for estimating the reliability of the optimal solution:

$$r = (S_{sz} - 1/2)/[S_{sz} + 2(\sigma_Y^2 + 1)] \tag{1}$$

where r is the reliability, S_{sz} is the stack size and σ_Y^2 is the variance of the log hydraulic conductivity. The reliability of the optimal solutions identified in that study for different stack sizes was reasonably well estimated using the formula. Based on the slow increase in reliability with respect to increase in stack size, as indicated by this formula, they concluded that large stack sizes ($\sim$1000) would be needed to achieve reliability very close to 1 (Feyen and Gorelick, 2004).

A solution to this issue of either a low reliability or a prohibitively large stack size to achieve reliable solutions is presented in this paper. The proposed method helps to identify high reliability solutions more efficiently compared to past methods and is demonstrated in this study using an injection bore field design problem. Additionally, focus is also on identifying robust solutions. Robustness is defined as the characteristic of the solution by which it is less sensitive to perturbations of uncertain parameters (Deb and Gupta, 2006). Robustness is different from reliability in this context. For example, considering a conservative estimate of the parameter field in the simulation–optimization may yield a reliable solution, but it does not necessarily be a robust solution. In this study, the single objective groundwater optimization problem is formulated in a stochastic multi-objective optimization framework to depict the trade-off between the optimal solution of the groundwater management problem and solution robustness, thereby defining a Pareto front. A Pareto front is defined by those solutions for which an improvement in one objective function is not possible without a reduction in another objective function (Deb et al., 2002). In our formulation, the first objective function defines the primary goal of groundwater management as would be used in a traditional single objective optimization. The second objective function is defined to minimize prediction uncertainty, which is quantified using prediction variance, consistent with other optimization formulations (Mulvey et al., 1995; Watkins and McKinney, 1995; Karatzas and Pinder, 1997; Ricciardi et al., 2007).

Evolutionary optimization using the population-based algorithms is ideally suited to explore solutions for single and/or multiple conflicting objectives of optimization (Aly and Peralta, 1999; Cheng et al., 2000; Park and Aral, 2004; Bhattacharjya and Datta, 2005; Qahman et al., 2005; Mantoglou and Kourakos, 2007; Sreekanth and Datta, 2011a,b, 2012; Valipour and Montazar, 2012a,b; Ketabchi and Ataie-Ashtiani, 2015; Gopalakrishnan and Kosanovic, 2015; Akca et al., 2014; Caldwell et al., 2013; Nourani et al., 2014; Luo et al., 2014). The multi-objective genetic algorithm NSGA-II (Deb et al., 2002) which has been popularly used in water resources literature (Park and Aral, 2004; Mantoglou and Kourakos, 2007; Sreekanth and Datta, 2010; Bau and Lee, 2011; Kourakos and Mantoglou, 2011, 2013) uses the population based approach to organize the candidate solutions into Pareto fronts. The Pareto-concept has recently been used for exploring conflicting management objectives of saltwater intrusion management in coastal aquifers (Sreekanth and Datta, 2010, 2014) and hypothesis testing using groundwater models (Moore et al., 2010). The NSGA-II algorithm defines the entire Pareto front from a single optimization run and does not require the use of an objective function weighting scheme. Hence NSGA-II was used for solving the multi-objective formulation developed in this study.

The optimization approach, implemented with the multi-objective framework developed herein, helps to achieve robust and reliable solutions for groundwater management. The proposed approach has the advantage that the robust and reliable solutions can be obtained by using lesser number of realisations of the model parameter fields than the multiple realization optimization schemes reported in the past. This helps in increasing the efficiency of the stochastic simulation–optimization method. Another advantage of this multi-objective stochastic optimization is the greater information on the trade-off between the optimal solutions and their respective uncertainty is made available to the decision maker, who traditionally adopts a precautionary approach in the context of prediction uncertainty. In a single objective high-reliability based optimization the trade-off between the optimal solutions and uncertainty is not revealed.

The paper is set out as follows. Section 2 briefly describes the synthetic groundwater management problem which is used to illustrate the developed method. In Section 3, the mathematical formulation of the optimization problem and implementation for the chosen example are presented. The results from a comprehensive analysis are presented and discussed in Section 4. The conclusions drawn from this numerical experiment are then summarized in Section 5.

2. Synthetic groundwater management example

There are a number of groundwater management problems where robust and reliable solutions are required to minimize the risk of undesirable outcomes resulting from a groundwater