Predictive uncertainty analysis with a Pareto method for a salt water intrusion model

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ABSTRACT

Predictive uncertainty analysis for salt water intrusion models can be a computationally demanding task. Recently, a Pareto front analysis was introduced to identify structural model defects and to assess the likelihood of extreme model predictions. Through exploration of such a Pareto front the optimal trade-off can be found between model misfit and a set of constraints on model parameters or model outputs. In this research a Pareto front analysis is applied for a synthetic salt water intrusion model, based on the Henry-problem. Results are compared with an uncertainty analysis performed with a Markov-Chain Monte Carlo method.

Keywords: *Pareto front, predictive uncertainty, Henry problem, salt water intrusion.*

INTRODUCTION

Salt water intrusion models are a common instrument to evaluate the impact of increased groundwater withdrawal and climate change on freshwater resources within coastal aquifers (Lebbe *et al.* 2008; Giambastiani 2007). In order to make decent predictions, these salt water intrusion models are often required to simulate a past system response. For this purpose these models are calibrated. However, when many parameters are involved, observation data is scarce and an accurate description of the modeled system is lacking, many different parameter sets can result in a physically acceptable model, which fits the measurement data. Ideally, predictions should be made with all these parameter sets. In practice this is often impossible due to computational limitations. Since saltwater intrusion models are highly nonlinear and the focus is merely on extreme prediction values, the application of a linear uncertainty method can be insufficient. In this case, methods like DREAM (Vrugt *et al.* 2009), GLUE (Beven and Binley 1992) and the Sub-Space Monte Carlo method (Tonkin and Doherty 2009) can be used to perform a more accurate prediction uncertainty analysis. An alternative to these methods could be a Pareto front analysis, which shows the trade-off between model misfit and parameters or model output constraints. To traverse the Pareto front efficiently for models that have already been calibrated the calibration software PEST (Doherty 2003) was used to move along such a Pareto front (Moore *et al.* under review). The method was applied to assess the likelihood of extreme prediction value for a synthetic salt water intrusion model. The method was also applied to determine appropriate weights for the different data types and the preferred parameter value constraints used during the model calibration. Finally the results are compared with an uncertainty analysis using the DREAM algorithm (Vrugt *et al.* 2009), which is based on a Markov chain Monte Carlo method.

MATERIALS & METHODS

The Pareto method was applied for a synthetic salt water intrusion model based on the well-known Henry problem (Henry 1964), which is widely used as benchmark for variable density codes (e.g. Voss and Souza 1987; Langevin *et al.* 2007; Essink 2001) and for testing new concepts in salt water intrusion modeling (Held *et al.* 2005; Sanz and Voss 2006). The setup was slightly modified, as a stochastic hydraulic conductivity field was used and two stress-periods, one for model calibration and a second one to predict the inland movement of the freshwater-salt water interface after reducing the incoming freshwater flux. All simulations were executed with SEAWAT (Langevin *et al.* 2007).
The random hydraulic conductivity field (Figure 1) was generated based on an exponential variogram with a sill of 0.1 and a range of 0.45 m. This hydraulic conductivity field defines the truth as far as this numerical experiment is concerned. Based on a simulation with this field, observation data, heads and concentrations, were generated for 12 observation points. The resulting prediction, the position of the 10% seawater line, associated with the "true" field was 0.77 m. Subsequently, the model is calibrated using 50 pilot-points (Certes and Demarsily 1991). To simplify the parameterization of the model preferred value regularization is applied, with preferred values equal to the mean used during the generation of the random hydraulic conductivity field.

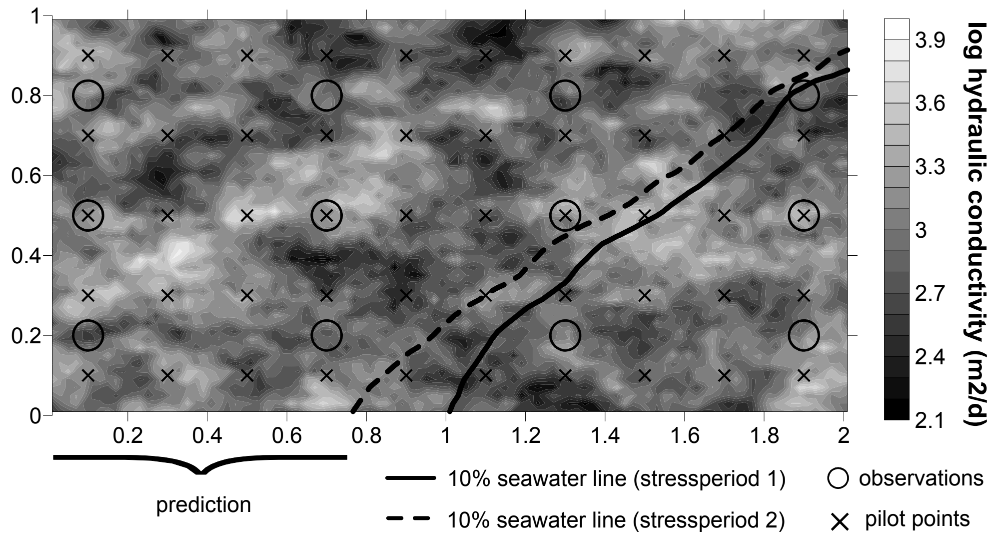

Figure 1 Stochastic hydraulic conductivity field, locations of pilot points and observation data. Position of the 10 % seawater line indicated before and after reducing the freshwater flux in stress period 2.

RESULTS

The calibrated model resulted in a prediction of 0.67 m. This is 0.1 m more inland compared to the truth of 0.77 m. Since the model fitted the observation data appropriately, this error reflects the inability of the calibration process to capture the details of the hydraulic property distribution. This calibrated model is the starting point for traversing the Pareto front in incremental steps by forcing the salt water intrusion model to satisfy a certain prediction value. This is done by assigning increasing weights to the prediction and a recalibration of the model for both the measurement data and the model prediction.

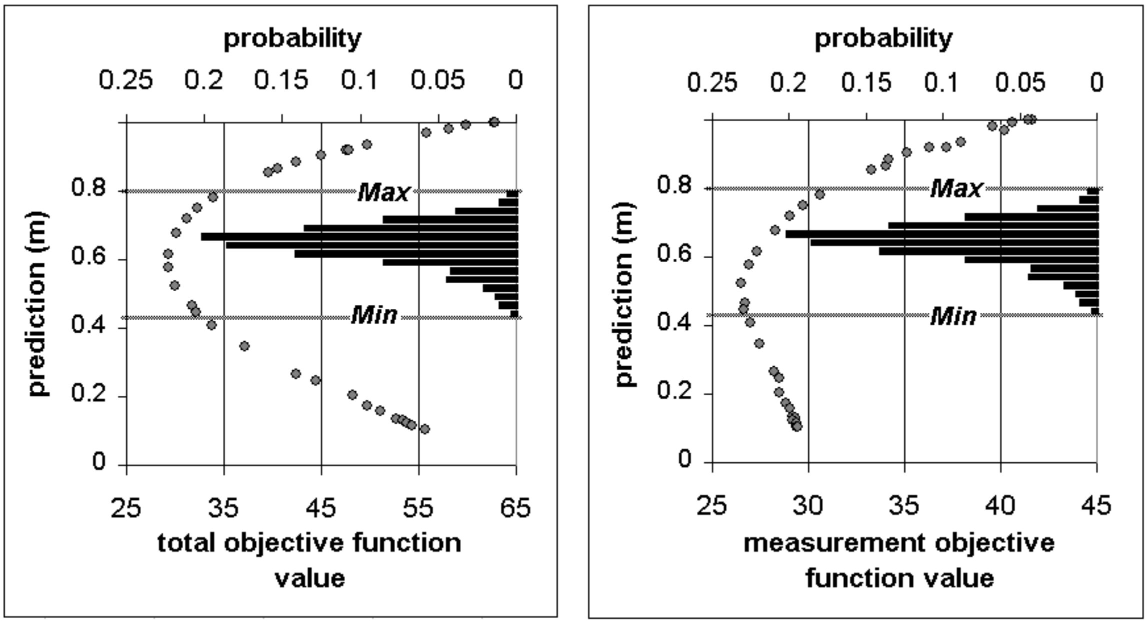

Figure 2 Prediction versus the total objective function value (left) and prediction versus the measurement objective function associated with the available concentration and head observations (right). Results of the uncertainty analysis with DREAM are indicated by the histogram and the lines Min and Max.

Figure 2 shows the Pareto front for the measurement objective function versus model prediction after approximately 2000 model runs. This amount of model evaluations does not indicate the efficiency of the method, since the number of model runs in which the Pareto front is traversed was chosen arbitrarily. The figure is subdivided for a measurement objective function with and without the preferred value regularization component. As can be seen the objective function starts to increase when the prediction is respectively increased and decreased to extreme values. The true prediction value of 0.77 m is located relatively close above the optimal point of the Pareto front. For very low prediction values, indicating extreme saltwater intrusion, the objective function mainly increases due to the regularization term, which means the hydraulic conductivity field becomes less physically acceptable in order to satisfy the low prediction values. After 20000 model evaluations DREAM provided 516 calibration constrained parameter sets. The minimum and maximum prediction values associated with theses sets are indicated in Figure 2 to compare with the Pareto front. These two bounds correspond fairly well with the prediction values, for which either the measurement objective function or the regularization objective function starts to increase more rapidly.

CONCLUSION

A Pareto-front analysis can offer valuable information regarding the probability of extreme salt water intrusion model predictions. Based on the objective function values associated with model misfit and prior parameter constraints, a measure for the likelihood of different model predictions can be obtained. For the synthetic model used in this research the results compared well with an uncertainty analysis with a Markov-chain Monte Carlo method. The true prediction value was located within the acceptable range of the Pareto-front. In a real-world modeling context, the assessment of predictive uncertainty with a Pareto front would be performed on a subjective basis. However, this method can be of particular interest for predictions with very small probabilities, since a

Pareto front is able to efficiently associate confidence limits with such predictions. Nonlinear uncertainty techniques, like Monte Carlo methods, would often require many more model runs to determine whether extreme model predictions are within the uncertainty bounds of a model.

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