MINI REVIEW

Environmental modeling in the towards of reproducibility

A M Wilson

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ABSTRACT

A completely functioning example of uncertainty quantification (UQ) and parameter estimate (PE) on a decision-support-scale is shown. The assessments are carried out using an existing groundwater flow model for the Edwards aquifer in Texas, USA, using a script-based methodology that aims to be transparent and repeatable. To history-match simulated outputs to corresponding state observations of spring flow and groundwater level, high-dimensional PE is applied. Then there's a back cast of a past drought. The combined UQ and PE studies are shown to generate an ensemble of model solutions that frame the observed hydrologic responses using accessible state measurements obtained under drought circumstances. All of the information and scripts used in the studies have been released into the public domain to serve as a model for other practitioners who want to perform similar work.

Key Words: *Aquifer; Horizontal flow barrier groundwater level; Variogram; MODFLOW*

INTRODUCTION

The value of uncertainty quantification (UQ) in environmental modelling for decision support is well understood Parameter estimation (PE) is also critical, which we define as the process of lowering uncertainty by historically matching simulation outputs to their state observation equivalents (a process sometimes referred to as "calibration"). UQ and PE, when combined, are key analyses for model-based resource management decision support because they offer estimates of uncertainty in important simulated outcomes and help to reduce that uncertainty. There are also considerable calls for modeling-based analysis (including UQ and PE assessments) to become more transparent, repeatable, and responsible. The reasons for this movement are self-evident; various organisations have campaigned for more transparency and reproducibility in computational science and environmental modelling. Some authors have provided examples of how the forward environmental model construction process might be made more reproducible. In order to strengthen the reproducibility of the forward model construction process, certain script-based tools for practitioners have been developed2016). In many situations, the necessity for PE and UQ can compete with the need for reproducibility.This is because PE and UQ analyses necessitate many more subjective conceptual choices and introduce many more operations and steps into the modelling analysis' implementation, and these added difficulties can significantly reduce a modelling analysis' reproducibility.

This loss of reproducibility, particularly in the results of the PE and UQ studies, might erode the model's credibility as a decision-making tool and stymie resource management efforts. We offer a script-based workflow for reproducible UQ and PE analysis in this paper. We use the term "reproducible" to refer to providing readers with the datasets and scripting tools they'll need to replicate the results. Based on the model, we employ an existing model of the Edwards aquifer in Texas, USA from the work [1]. The model is a MODFLOW-2005 model with 1 layer, 370 rows, and 700 columns arranged on a regular grid with a spacing of 1,340 feet; the model domain's geographic location; and the features of interest. The Recharge (RCH) package simulates both diffuse and concentrated recharge processes in the model domain. Spring flow (simulated with the Drain (DRN) package) and extraction wells (simulated with the Well (WEL) package) are two ways in which water escapes the model domain. The Horizontal Flow Barrier (HFB) package is used to describe faults that are expected to behave as flow barriers. The model has been divided into two time periods for simulation:

- Monthly stress periods are used to recreate the period 2001–2015 in a history-matching simulation
- Scenario simulation: mimics the period 1947–1958 (known as the "drought of record") with monthly stress periods for PE

Editor office, Journal of Environmental Geology, United Kingdom.

Correspondence: A M Wilson, Editor office, Journal of Environmental Geology, United Kingdom, e-mail id environgeol@journalres.com

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(i.e., history matching) of observed spring flows and groundwater levels; This simulation is used to backcast simulated conditions of key importance to groundwater resource managers, such as spring flow at Comal and San Marcos springs and groundwater level at index wells J-17 and J-27. Groundwater levels at index wells J-17 and J-27 during the scenario (e.g., drought) simulation are of particular significance to groundwater resource management and are the primary focus of the UQ and PE analyses reported herein [2]. As a result, throughout the history-matching simulation, we focus the PE analysis on duplicating the observed spring flow and water levels as accurately as possible. Replicating these observed states during history-matching should, logically, increase the ability to reproduce these observed states during scenario simulation. At the Comal and San Marcos springs, as well as index wells J-17 and J-27, state data of spring flow and groundwater level are also available for the scenario hind cast simulation. The uncertainty in parameters and outcomes of major interest to groundwater resource managers is represented using a Bayesian uncertainty framework in this paper. The definition of the Prior is an important aspect of any Bayesian uncertainty quantification (UQ) investigation. We use a high-dimensional parameter space to get reliable estimates for the hindcast of simulated states of major importance to groundwater resource managers, while also striving to prevent under-parameterization Knowling effects. In the history-matching and scenario simulations, we employed 337,482 and 339,449 parameters to reflect model input uncertainty. Both simulations use the identical static (i.e., time-invariant) attributes of hydraulic conductivity, storage, HFB conductances, and DRN boundary elements (stage and conductance). This is PE's mechanism for reducing uncertainty in scenario-simulation outcomes that are of main concern to groundwater resource managers. If these outputs are sensitive to static properties and the static properties' uncertainty is reduced by PE, the scenario-simulation outputs' uncertainty may be lowered as well.

We employ a multi-scale parameterization technique (2019) to clearly represent distinct spatial dimensions of uncertainty in the PE analysis, as well as to aid understanding of how information is transmitted from observable states to parameters (at various sizes). Three spatial scales of parameterization were employed for hydraulic conductivity, particular storage, specific yield, and beginning conditions:

• a single multiplier parameter that applies to the entire domain ("global") grid-scale multiplier parameters at a spacing of 39,600 feet.
• pilot point multiplier parameters at a spacing of 39,600 feet (one parameter per active computational cell).

Recharge was controlled with time-varying domain-wide multiplier parameters and time-varying multiplier parameters for each of the 25 recharge "zones"—a domain-wide multiplier parameter and a multiplier parameter for each zone were set for each stress period. We are attempting to account for both spatial and temporal uncertainty in the recharge estimations in this manner [3].

• At a spacing of 39,600 feet, pilot point multiplier parameters and grid-scale multiplier parameters (one parameter per active computational cell). We can account for both spatial and temporal uncertainty in the recharge estimations. The Edwards aquifer recharge estimation process and provides an example of recharge zonation. The multi-scale parameterization is graphically summarized in the Supplementary Material, which is recommended to readers. The rates of well extraction were also adjusted to take to consideration spatial and temporal variations. The well extraction rate estimations were additionally parameterized to allow for spatial and temporal uncertainty in the estimates. Throughout all stress periods, a single set of extraction rate multiplier settings (one per well) was used. This collection of spatially distributed multiplier parameters was combined with a set of temporally distributed multiplier parameters to create a new set of multiplier parameters (one for each stress period). While groundwater extraction rates were metered during the history-matching phase, the model's simulated groundwater extraction is still uncertain due to uncertainty (e.g., error) generated by spatial and temporal discretization. The above-mentioned UQ and PE analyses were carried out using a python-based scripting workflow; the process is wholly included within the python script eaa.py and is implemented as functions within this script. The basic history-matching and scenario simulation model input files are left "as-is," with the scripting process handling the rest. The workflow follows these phases at the highest level (function names are in parentheses):

(Setup models parallel): Generate a high-dimensional PEST interface by processing the model input files for both history-matching and scenario simulations. Programmatically adjusting the MODFLOW model input formats to allow free-format and external files, as well as rectifying the WEL files so that the same number of well entries appear in each stress period, which is critical for parameterizing well extraction rates, are among the tasks. For consistency, include additional extraction well entries with an extraction rate of zero. Using the Prior distribution, define the geostatistical prior parameter covariance matrix and build prior parameter ensembles of 100 realisations for each simulation. 13 realisations were removed from the history-matching simulation prior parameter ensemble due to long run times, and 5 realisations were removed for yielding "dry" model cells for locations where groundwater levels were measured, leaving 82 realisations for the PE analysis [4]. These 82 realisations were used to evaluate prior and posterior scenario simulation uncertainty.

The scenario simulationwas examined 182 times, whereas the history-matching simulation was reviewed 310 times. The pre and posterior ensembles, in general, bracket the observed states behaviour for both history-matching and scenario simulations at the four major areas of concern to groundwater resource managers. The observed states at the four locations of key relevance to groundwater resource managers are densely clustered in the posterior ensemble. At the four locations, the scenario simulation posterior ensemble does not produce the same amount of reproduction. This is due to the inclusion of scenario-specific recharge and well-extraction uncertainty, which are expressed as parameters that only appear in scenario simulations. That is, regardless of how much the static characteristics are conditioned during history-matching simulation PE analysis, these scenario-only parameters maintain their prior uncertainty, causing uncertainty in the scenario posterior simulated outputs [5]. The combined UQ and PE analyses are likely to be robust at hindcasting (in a stochastic sense) the hydrologic response to drought at these four locations, as the posterior scenario simulation ensemble brackets the observed low spring-flow rates and low water levels at the springs and index wells of primary interest to groundwater resource managers. This is a positive result, indicating that the automated procedure is performing as planned. This success can be attributed to the use of a high-dimensional parameter space (which helps to avoid under-estimation of uncertainty and limits the potential negative effects of model error), as well as a likelihood function that was focused on outcomes of primary interest to groundwater resource managers [6].

For both the history-matching and scenario simulations, we compared the residual L2 norm () at the four locations of key importance to groundwater resource managers. Even though the scenario simulation outputs were not used in the PE analysis, we can observe that the PE analysis was able to minimize for both the history-matching and scenario simulation ensembles. We also see that the posterior values for some realisations are lower than the previous models. The reduction in under scenario settings is due to the ensemble learning about the static features in the history-matching simulation and then transferring these static properties to the scenario simulation via PE. The script-based analysis, such as the one described here, will be error-free. The vast number of operations and decisions required shows that there are problems or "bugs" in the script (and underlying modules) used to implement these analyses in a statistical sense—the normal fault rate in production-level software is between 15 and 50 faults per 1,000 lines. Unlike non-scripted modelling workflows, however, these "faults" can be identified and investigated by other practitioners long after the analysis has been completed—all of the assumptions, decisions, and operations required to implement our analysis are transparently encoded in the scripting workflow [7]. In other sectors, such as some omics cancer research, where the ramifications of data processing decisions might have life or death consequences, this level of transparency and reproducibility has become a prerequisite. Furthermore, once faults are detected, they can be corrected programmatically in the script, allowing the UQ and PE analyses to be re-run from start to finish without the added complexity of creating new flaws. While the initial "investment" to establish the scripting workflow is significant, the returns on investment, as evaluated by efficiency and integrity, are significant.

CONCLUSION

The PE approach in PESTPP-IES has been found to support very high-dimensional history matching at a low computing cost—the PE analysis took around 300 model evaluations, while the scenario prior and posterior Monte Carlo runs each took about 100 model evaluations. This efficiency allows practitioners to focus on expressing model input uncertainty as strongly as feasible rather than how model inputs are specified in the context of a computational trade-off. Given the interest of groundwater resource managers in the hydrologic response to drought and the availability of state observations for PE have also been subjected to PE.

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