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Global sensitivity analysis and calibration of parameters for a physically-based agro-hydrological model

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ABSTRACT

Efficient parameter identification is an important issue for mechanistic agro-hydrological models with a complex and nonlinear property. In this study, we presented an efficient global methodology of sensitivity analysis and parameter estimation for a physically-based agro-hydrological model (SWAP-EPIC). The LH-OAT based module and the modified-MGA based module were developed for parameter sensitivity analysis and inverse estimation, respectively. In addition, a new solute transport module with numerically stable schemes was developed for ensuring stability of SWAP-EPIC. This global method was tested and validated with a two-year dataset in a wheat growing field. Fourteen parameters out of the forty-nine total input parameters were identified as the sensitive parameters. These parameters were first inversely calibrated by using a numerical case, and then the inverse calibration was performed for the real field experimental case. Our research indicates that the proposed global method performs successfully to find and constrain the highly sensitive parameters efficiently that can facilitate application of the SWAP-EPIC model.

1. Introduction

Agro-hydrological models have been an important tool for supporting decision making in the development of agricultural water management strategies. Since the physical description and prediction of hydrological, chemical and biological processes at field by some physically-based or mechanistic models are highly valuable, these models, such as SWAP (van Dam et al., 1997) and HYDRUS (Šimůnek et al., 1997), are frequently used. Most of them are based on the numerical solution of Richards equation for variably saturated water flow and on analytical or numerical solution of advection-dispersion equation. Compared with the simple models (i.e. using lumped or tipping-bucket approach, e.g. SIMdualKc, AquaCrop, CERES and EPIC), these mechanistic models can simulate multi-processes of soil water flow, solute and heat transport, and crop growth in great detail, and be suitable for some more complicated conditions (Ranatunga et al., 2008; van Dam et al., 2008; Xu et al., 2013). However, these models often contain more number of parameters, and have complex, dynamic, and nonlinear properties. Moreover, more functions have been added involving hysteresis, mobile-immobile flow, macropore flow, multi-species transport and reaction, and so on. These may result in a more severe problem of over-parameterization. Hence, the parameter identification becomes a major and urgent problem for agro-environmental prediction and future model use (Ines and Mohanty, 2008; Wöhling et al., 2008; Della Peruta et al., 2014). An efficient identification of the sensitive and important parameters and the subsequent parameter estimation would be very helpful for the future use of physically-based agro-hydrological models.

Parameter sensitivity analysis (SA) is a prerequisite step in the model-building process (Campolongo et al., 2007). The SA method identifies parameters that do or not have a significant impact on model simulation of real world observations for specific farmlands (van Griensven et al., 2006) and is critical for reducing the number of parameters required in model validation (Hamby, 1994).

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Generally, SA can be divided into two different schools: the local SA school and the global one (Saltelli et al., 1999). In the first approach, the local response of model output is obtained by varying the parameters one at a time while holding the others fixed to certain nominal values. This approach has been adopted by some studies because of its easy application. Yet, local SA methods have the known limitations of linearity and normality assumptions and local variations. For complex non-linear models, only global sensitivity analysis (GSA) methods are able to provide relevant information on the sensitivity of model outputs to the whole range of model parameters (Varella et al., 2010). In recent years, many studies have focused on the GSA methods for identifying the important parameters as well as distinguishing the effects of different input conditions (Wesseling et al., 1998; Cariboni et al., 2007; Saltelli and Annoni, 2010; DeJonge et al., 2012; Zhao et al., 2014; Neelam and Mohanty, 2015; Hu et al., 2015; Pianosi et al., 2015). Typical successful applications include the methods of RSA (Yang, 2011), extended FAST (Varella et al., 2010), Sobol' (Nossent et al., 2011) and LH-OAT (van Griensven et al., 2006) in the related hydrological and crop models. The choice of the sample size and of the threshold for the identification of insensitive input factors was also preliminarily investigated for GSA methods (Yang, 2011; Sarrazin et al., 2016). Although different sensitivity techniques exist, each of them would result in a slightly different sensitivity ranking for the important parameters near the top of the ranking list. In general, the practicality of the method depends on the calculation ease and the desired usefulness of results (Hamby, 1994).

Parameter estimation is an essential way of calibrating a model, which is also important to the accurate prediction of agro-hydrological processes. Different approaches have been applied and may be classified as two main types, i.e., trial-and-error method (manual) and inverse optimization method (automatic). The former has been widely applied because of its simple concept and easy application (Xu et al., 2013). It is very suitable to the simple models with less parameters and complexity, such as when applying to the SimDualKc and AquaCrop models (Paredes et al., 2014). However, the trial-and-error method is often cumbersome and time-consuming when applying to the physically mechanistic models, especially for layered soil-profile and complicated field conditions (Jacques et al., 2002). Hence, in addition to the subjectivity of the trial-and-error method, there have also been a large number of research studies on its alternative: automatic inverse optimization approaches for model calibration. These algorithms may be classified as local and global search methods. The local method, using an iterative search starting from a single arbitrary initial point, may often prematurely terminate the search and therefore present a lower chance to find a single unique solution, such as the well-known Gauss-Marquardt-Levenberg algorithm used by PEST (Wöhling et al., 2008; Malone et al., 2010). This inspires the application of global parameter estimation (GPE) methods in the field of vadose zone hydrology, e.g., genetic algorithms (Ines and Droogers, 2002; Ines and Mohanty, 2008; Shin et al., 2012), ant-colony optimization (Abbaspour et al., 2001), Ensemble Kalman Filter (Evensen, 2003) and shuffled complex methods (Duan et al., 1994). In the past, the inverse optimization of parameters of soil hydraulic properties as well as the related well-posedness, uniqueness and the stability are extensively studied related to the physically-based models (Kool et al., 1987; Šimůnek and van Genuchten, 1996; Ines and Droogers, 2002; Shin et al., 2012). The inverse estimation of root water uptake parameters is also carried out (Hupet et al., 2003). In contrast, very few research studies extend to simultaneously consider the solute fate simulation and its parameter estimation (Jacques et al., 2002; Xu et al., 2012). Note that they are of importance for the accurate agro-hydrological modeling in salt-affected irrigated areas, where the ignorance of solute transport would lead to errors in the inverse parameter estimation. Uncertainty analysis is also applied in watershed hydrological modeling (Yang et al., 2008), but only a few cases are related to the detailed and complicated field scale studies (Shin et al., 2012; Shafiei et al., 2014).

To our knowledge, few studies have reported the development of both parameter sensitivity analysis and inverse estimation for the complicated physically-based agro-hydrological models. The general purpose of this study was to investigate the global method of sensitivity analysis in conjunction with inverse parameter estimation for effectively identifying parameters of a mechanistic agro-hydrological model (SWAP-EPIC). SWAP-EPIC is modified version of the well-known SWAP model, proposed by Xu et al. (2013). A GSA module and a GPE module were respectively developed for SWAP-EPIC model to perform sensitivity analysis and estimation of model parameters. An efficient Latin Hypercube One-factor-At-a-Time (LH-OAT) method was adopted to construct the GSA module. The GPE module was then developed based on the genetic algorithm (GA). Meanwhile, to avoid the problem of numerical instability, a new solute transport module was developed with the fully implicit and Crank-Nicholson difference schemes. Finally, the proposed global method for sensitivity analysis and parameter estimation was tested and verified using the field experiment datasets in Huinong experimental site, Qingtongxia Irrigation District of the upper Yellow River basin, Northwest China. The methodology described in this study would help increase the efficiency of parameter identification for the complicated agro-hydrological model and would also help understand the relationship between different processes.

2. Materials and methods

2.1. Model description

2.1.1. Agro-hydrological simulation model: updated SWAP-EPIC

By coupling the SWAP (Soil-Water-Atmosphere-Plant) model (Kroes and van Dam, 2003) and the EPIC crop growth module (Williams et al., 1989), Xu et al. (2013) proposed an agro-hydrological simulation model SWAP-EPIC. This model had been used to evaluate soil water flow, solute transport, crop growth, and water productivity in Heihe River basin (Jiang et al., 2015) and Yellow River basin (Xu et al., 2013, 2015). However, based on our experience, the numerical solution of solute transport is not stable enough in original SWAP-EPIC with the explicit finite-difference scheme, because the time step should meet the stability criterion for ensuring stability (van Genuchten and Wierenga, 1974). When the size of time step exceeds a limit and stability criterion is not satisfied, the numerical errors in the solution are amplified as the time marches forward, leading to an invalid or unstable solution (Zheng and Bennett, 2002). According to our experience, this caused very large numerical errors and mass imbalance for salinity problems in SWAP-EPIC, which was prone to happen in GSA and GPE modeling with a large range of parameter changes (Xu et al., 2012, 2013). Subsequently, it would lead to the crash of GSA simulation and efficiency reduction for GPE simulation. Therefore, in this study, we developed a new solute transport module optionally using the fully implicit or Crank-Nicholson finite-difference scheme to replace the original one in the updated version of SWAP-EPIC. It could indeed improve the model stability and make the calculation much faster. Main processes of the modified SWAP-EPIC model are described below.