Global sensitivity and uncertainty analysis of nitrate leaching and crop yield simulation under different water and nitrogen management practices

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\textbf{Abstract}

Assessing the sensitivity and uncertainty of soil-crop models is beneficial to model calibration and development of best water and N management practices. This study adopted the Morris screening method and the Sobol’ variance-based method, combined with an agricultural system model (WHCNS), to analyze the global sensitivity and uncertainty of nitrate leaching and crop yield to model input parameters under different water and N management practices. A two-year field experiment was conducted in a desert oasis of Inner Mongolia, China using a factorial combination of standard (I\textsubscript{std}, standard, 750 mm per season; N\textsubscript{std}, standard, 138 kg N ha\textsuperscript{-1}) and conservation (I\textsubscript{csv}, conservation, 570 mm per season; N\textsubscript{csv}, conservation, 92 kg N ha\textsuperscript{-1}) levels of irrigation and N fertilization: I\textsubscript{std}N\textsubscript{std}, I\textsubscript{std}N\textsubscript{csv}, I\textsubscript{csv}N\textsubscript{std} and I\textsubscript{csv}N\textsubscript{csv}. Sensitivity analysis (SA) based on this experiment showed that nitrate leaching demonstrated significant sensitivity to soil hydraulic and crop parameters, but generally low sensitivity to N transformation parameters. Based on Sobol’ SA, crop parameters accounted for 64.3%, 63.2%, 39.2% and 39.2% of simulated nitrate leaching variability for the I\textsubscript{std}N\textsubscript{std}, I\textsubscript{std}N\textsubscript{csv}, I\textsubscript{csv}N\textsubscript{std} and I\textsubscript{csv}N\textsubscript{csv} treatments, respectively. The greater the crop water and N stress, the stronger the parameters interaction. Uncertainty analysis showed the average amount of nitrate leaching under I\textsubscript{std} (135.3 kg N ha\textsuperscript{-1}) to be 2.3 times greater than under I\textsubscript{csv} (58.0 kg N ha\textsuperscript{-1}); however, the distributions of yield between the four treatment combinations did not show significant differences. Overall, irrigation practice was the main factor influencing the parameter sensitivities and the uncertainty of nitrate leaching and crop yield simulation. © 2017 Elsevier B.V. All rights reserved.

\section{1. Introduction}

In order to obtain high crop yield, farmers in China have applied excessive water and nitrogen (N) fertilizer, which has led to serious environmental problems, such as gaseous N emission (N\textsubscript{2}O and NH\textsubscript{3}) and nitrate contamination of groundwater (Hu et al., 2005; Gu et al., 2013). Nitrate leaching is an extremely complex process involving soil physical, chemical and biological processes, as well as their interaction with crops. As existing field-scale nitrate leaching measurement methods are time-consuming and generally of limited accuracy, many researchers have come to rely on soil-crop system models to quantify nitrate leaching (Hu et al., 2010; Qi et al., 2012; Wang et al., 2016). However, those models generally require many input parameters, making it difficult to calibrate adequately, and leading to significant uncertainty (Varella et al., 2010; Stella et al., 2014). A sensitivity analysis (SA) can be used to quantify the influence of each parameter on the variability of the model’s outputs and is therefore a key step to understand model performance in response to changes of these factors (Cariboni et al., 2007; Confalonieri et al., 2010). SA is useful in identifying low-impact parameters that may be converted to fixed values to simplify the model, as well as high-impact parameters to focus on during calibration or when a model is being used to evaluate agricultural policy (Vanuytrecht et al., 2014). The results of SA depend on the environmental conditions under which the model is run, e.g., climatic region, soil type and precipitation patterns, etc. Thus, altering environment conditions is crucial to examining the model’s general sensitivity (Confalonieri et al., 2010).

To evaluate model sensitivity to input parameters, local and global SA techniques (LSA and GSA, respectively) are typically used (Cariboni et al., 2007; Confalonieri et al., 2010). LSA investigates...
the effect of single input parameters on model outputs, while all other inputs remain constant. However, LSA is inapplicable to non-linear models (Cariboni et al., 2007; Saltelli et al., 2000). In contrast, GSA examines the average response of the model outputs when all parameters are simultaneously varied within defined ranges. This powerful technique considers parameter interactions and non-linear responses, but as it requires multiple model runs for parameter values varying over the parameter space, and it is computationally demanding (DeJonge et al., 2012; Vanuytrecht et al., 2014; Qin et al., 2016). The GSA techniques include screening methods and the variance-based methods. The screening method proposed by Morris (1991) identifies a limited set of influential parameters among all model parameters. The variance-based method (such as Sobol’; Fourier Amplitude Sensitivity Test, FAST; or Extended FAST, EFAST) decomposes the model output variance according to the influence of each contributing parameter (Saltelli et al., 2000). It determines not only the individual effect of a parameter, but also quantifies potential interactions among parameters. A GSA screening method is usually employed to reduce the computing needs of a more robust variance-based method (Vanuytrecht et al., 2014).

Recently, some studies adopted the GSA approach for soil-crop modeling (Varella et al., 2010; DeJonge et al., 2012; Vanuytrecht et al., 2014; Zhao et al., 2014; Qin et al., 2016; Liu et al., 2016). Varella et al. (2010) conducted SA and uncertainty analysis (UA) for the STICS model under 16 different configurations in soil, climatic and crop, and developed a tool to evaluate the performance of parameter estimation for those observation datasets. DeJonge et al. (2012), using both the Morris and Sobol’ methods, studied the response of CERES-Maize crop outputs (flowering, maturity, leaf area index, evapotranspiration, and yield) to crop parameters under different irrigation treatments, and proposed a new methodology for systematic calibration of CERES-Maize based on sensitivity indices for different treatments. They also found that screening method results from Morris were highly correlated with variance-based results from Sobol’. Vanuytrecht et al. (2014) studied the response of AquaCrop-predicted crop yield to various climate-crop-soil combinations using Morris and EFAST methods, and reported that the sensitivity of parameters depended on environmental conditions. Zhao et al. (2014) streamlined the calibration of APSIM using a GSA method, and concluded that to minimize cultivar-related uncertainty, cultivar parameters should be carefully calibrated when applying the APSIM-wheat model to a new cultivar under a new environment. Qin et al. (2016) and Liu et al. (2016) analyzed the uncertainty of soil organic carbon (SOC) simulation by DNDC and CENTURY models, respectively, using Sobol’ method, and identified the high sensitivity parameters to SOC dynamics. However, there were no studies that have applied the GSA method to assess the risk of nitrate leaching combined with crop yield simulation under different water and N fertilization management scenarios, or analyzed the parameters interaction under different crop water and N stresses.

On the other hand, a process-based soil-crop system model (soil Water Heat Carbon Nitrogen Simulator, WHCNS) was recently developed and has been successfully applied to analyze the effects of water and N management practices on nitrate leaching and crop yield in North China (Li et al. 2015; Liang et al. 2016a, 2016b). However, the parameter calibration of WHCNS is time-consuming and inaccurate due to lack of results in sensitivity analysis, which significantly limit the application of the model. Thus, the objectives of this study are to (i) evaluate the response of nitrate leaching and crop yield to soil hydraulic, crop and N transformation parameters using Morris and Sobol’ methods based on WHCNS model, and thereby identify the sources of uncertainty for the simulation of nitrate leaching; and (ii) analyze the risk of nitrate leaching and crop yield under different water and N management scenarios on the basis of Sobol’ uncertainty analysis.

2. Materials and methods

2.1. Field experiment

The field experiments were conducted in Alxa, Inner Mongolia, China (37°24′41′52″N, 103°21′106″51′E), with elevation ranging from 800 to 1500 m. The soils consisted of alluvium mixed with gray desert soils. The region is classified as warm-temperate typical desert arid zone with a continental climate. The mean annual precipitation is 116 mm, and the mean annual temperature is 8.3°C. Mean total potential evaporation reaches 3005 mm yr⁻¹, approximately 20 times the mean annual precipitation. The mono-cropping systems is planted in the middle of April and harvested in early October. The main crops are maize and spring wheat, which account for 80% of the cropped area.

The field experiments were conducted from April 2008 to October 2009, encompassing two spring maize production periods. Two irrigation treatments (Istd, standard irrigation, 750 mm per season; and Icsv, conservation irrigation, 570 mm per season) were factorially combined with two N fertilization treatments (Nstd, standard fertilization rate, 138 kg N ha⁻¹; Ncsv, conservation fertilization rate, 92 kg N ha⁻¹), resulting in four irrigation-fertilization treatments: IstdNstd, IstdNcsv, IcsvNstd and IcsvNcsv. Detailed information on water and N management practices for all treatments is shown in Table 1.

2.2. Data collection

The basic soil properties were measured in the top 1.8 m of the soil profile and are shown in Table 2. Soil volumetric water content (θ) was measured weekly at 20 cm intervals. Soil nitrate concentration was measured at seven key plant development stages. Crop dry matter at key plant development stages and yield were also measured, with the detail measurement methods described in Liang et al. (2016b). Meteorological data including daily minimum and maximum air temperatures, solar radiation, relative humidity, and wind speed were obtained from the Gila River weather station, located 45 km from the study area. Rainfall was measured on-site.

2.3. WHCNS model

The agricultural system model (WHCNS) was used to simulate soil water movement, soil heat and N transport, and crop growth. In the model, the reference evapotranspiration is estimated using the Penman-Monteith method (Allen et al., 1998). The infiltration of rainfall or irrigation is computed by a modified Green-Ampt approach (Green and Ampt, 1911). Water redistribution in the soil profile is simulated using the Richards equation in which plant water uptake is considered as sink. Runoff is calculated using the SCS curve number method proposed by the U.S. National Resource Conservation Service (NRCS, 2004). Meanwhile, the soil heat transport component is directly imported from the HYDRUS-1D model (Simunek et al., 1998). Soil C and N cycle algorithms are taken from the DAISY model (Hansen et al., 1990). Crop development, LAI, dry matter production and dislocation, and light-temperature potential production are simulated using the improved version of the PSi23 model which originated from the Netherlands (Driessen and Konijan, 1992). The water stress factor is defined as the ratio of the actual transpiration to the potential transpiration. The N stress factor is calculated based on the simulated crop N demand, actual soil N supply, and crop N uptake. The model runs on a daily time step and is driven by meteorological and crop biological infor-
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