A global uncertainty and sensitivity procedure for the assessment of groundwater recharge distribution via hydrological models

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Abstract Groundwater recharge is the key driver for groundwater flow and resulting transport at the catchment scale, but it is difficult to quantify. Hydrological models provide an option for evaluating an estimate of groundwater recharge. They can generally be used to estimate groundwater recharge rates over large spatial and temporal scales, and they can be applied for current or future scenario analysis as climate or land use changes. However, a serious limitation of current model applications is the non-availability of data and input parameters. In order to improve the reliability and the performance of hydrological models, in this study a general approach for the assessment of performance in the simulation of the groundwater recharge estimation is proposed. A so-called global uncertainty analysis is developed as a tool to evaluate the performance of the models. A global sensitivity analysis is defined and used as a complementary tool to find the most important sources of uncertainty. The procedure can take various sources of uncertainty into account, i.e. input data, parameters, either in scalar or spatially distributed form. This procedure is iterated in a loop for improving the performance of the models and to optimize the resource allocations. As a test example, the procedure is applied at an experimental site in northern Germany on a field scale, using the SWAP model, a 1D physical-based hydrological model. Further research will involve other spatially distributed hydrological models of different complexity and application on larger spatial scales.

Key words groundwater recharge; Richards equation; global sensitivity analysis

INTRODUCTION

The estimation of groundwater recharge, here taken as the vertical water flux below the root zone, is a critical issue for water resources assessment and for contaminant transport. Location and timing of groundwater recharge is dominated by several factors such as climate, geomorphology (including topography, vegetation and soil) and geology. Due to the complexity of the system and the interactions of all the compartments involved, the process is characterized by high spatial and temporal variability; therefore, a correct quantification of groundwater recharge is still a challenge for the hydrology sciences (Scanlon *et al*., 2002).

When the groundwater recharge is dominated by deep percolation from the unsaturated zone, a modelling approach is a common technique used to estimate the recharge in response to the meteorological forcing and the characteristics of the system. Recent advances in computer technology and computer codes made long-term simulations more feasible. A variety of approaches are now available, e.g. bucket models (e.g. Facchi *et al*., 2004), quasi analytic approaches (Simmons & Meywer, 2000) and numerical solution of Richards' equation (e.g. Tiktak *et al*., 2002; Twarakavi *et al*., 2008).

However, recharge estimation based on unsaturated-zone modelling may be highly uncertain due to the large amount of information needed to run the models. The data availability for setting up models is still indeed a critical issue and many limitations on the applicability of these models are considered in practical studies (e.g. Sivapalan, 2003). However, the assessment of the model performance is mostly carried out based on just the uncertainty of the soil parameters or with a one-at-a-time (OAT) method, so called as each factor is perturbed in turn, while keeping all other factors fixed at their nominal value (e.g. Jimenez Martinez *et al*., 2010). Even if these studies help the understanding of the system and the model behaviour, the conclusions in most of the cases are quite site specific and not useful for a global assessment of the model. Considering a more general approach for practical application, all the sources of uncertainty (i.e. input, parameters and model structure), have to be considered (Beven, 2007).

In this paper, a general probabilistic framework for the uncertainty and sensitivity analysis of hydrological models is used considering the problems mentioned above. In this framework all the sources of uncertainty can be explicitly considered without any constraint, e.g. using spatially distributed parameters or input or different models. This framework is based on the approach proposed by Crossetto & Tarantola (2001) and recently revisited in Lilburne & Tarantola (2009). In this paper, the framework is used with SWAP model (Kroes & Van Dam, 2003), a 1D physically-based hydrological model, for the estimation of the groundwater recharge in a cropped field located in Bornim (Brandenburg, Germany). However, the proposed framework is readily extendable to a wide variety of distributed hydrological modelling applications.

METHODS

The general probabilistic framework

The general framework proposed for the uncertainty and sensitivity analysis is based on a Monte-Carlo simulation and the variance-based approach (Saltelli *et al*., 2006). Here, once the distributions of the input factors are defined, the model runs are iterated for each possible realization created and the variance of the models output is calculated. The sensitivity indexes considered are the so-called First sensitivity index (S_i) and Total sensitivity index (S_T) as follows:

$$S_i = \frac{V[E(Y \mid X_i)]}{V(Y)} \tag{1}$$

$$S_T = \frac{E[V(Y \mid X_{\sim i})]}{V(Y)} \tag{2}$$

where the first index is the ratio between the variance of the mean output Y conditioned by all the possible X_i input values and the total variance of the output $V(Y)$. The higher S_i is, the higher the importance of the input factor i is. In the case of the second index, this ratio S_T considers variance of the mean output Y is conditioned by all the possible input values except X_i. The lower S_T, the lower the importance of the factor X_i is. Differences in the two indexes indicate the interaction of the input factors considered in the analysis. For more details see also Saltelli *et al*. (2000).

In the specific framework proposed here, all sources of uncertainty in the study can be considered, because the sensitivity analysis is based on the simple introduction of a trigger factor used to randomly select the samples that have to be considered. This approach was applied for example by Crosetto & Tarantola (2001), who proposed the use of a sensitivity analysis of a binary input to “switch” uncertainties on and off at the same rate (i.e. for N/2 runs, the switch is set to off and for the remaining N/2 runs it is set to on), allowing their relative importance to be determined. The same approach was applied by Lilburne *et al*. (2003), who associated sampling values from a discrete, uniformly-distributed input, with sample realizations from a pre-generated sequence of 1000 realizations of a set of soil maps. This enabled a complex correlated description of variability in soil profile data to be simulated, which was not possible with other more common approaches.

The estimation of the sensitivity indexes is subsequently done based on the variance decomposition proposed by Sobol (2001) and further developed by Saltelli (2002). As shown by Tang *et al*. (2007), this method yields more robust sensitivity rankings than other measurements such as the analysis of variance or regional sensitivity analysis. Moreover, with this method an analytical model to link input and output is not required, because the estimation of the sensitivity indexes does not depend on the order in which the realizations are associated with the scalar input values. For more details about the method see Lilburne & Tarantola (2009).

Experimental site and data collected

The model application is conducted for a cropped flat field of 30 ha located in Bornim (Brandenburg, Germany), where surface runoff can be neglected and the 1D vertical fluxes play the most important role. The area situated 40 m a.s.l. is characterized by loamy-sand soil (Gebbers *et al*., 2009), a mean annual precipitation of 595 mm and minimum and maximum temperatures of –15ºC (February) and 30ºC (July), respectively (Meteorological Station Potsdam Telegrafenberg, Germany). The study was conducted for May–August 2011, and is focused on the temporal variability of evapotranspiration, soil moisture in the root zone, and recharge simulated by the model. The model performance is evaluated considering the variance of the model outputs due to evapotranspiration and recharge. The performance of the soil moisture dynamic simulated was compared with soil moisture measured by Theta Probes (Delta-T Devices, Cambridge, UK) installed in the field at three depths (0, 20 and 40 cm). In this case the mean error, ME (-), between simulated and measured mean soil moisture in the root zone (50 cm) is calculated for the period considered. For more details of the experimental site see Rivera Villarreyes *et al*. (2011). During the season, monitoring activities were also conducted in order to collect the input and parameters to set up the model and to define the uncertainty in the data available. In particular, meteorological data (i.e. temperature, air humidity, solar radiation, wind velocity and precipitation) were available from the Meteorological Station Potsdam Telegrafenberg. However, the station is located approximately 6 km east of the experimental site. Direct measurements in the field were also collected during the season and compared to the reference in order to define the range of uncertainty for each variable. In 2011 the field was cropped with sunflowers. Crop parameters to set up the model were based on Allen *et al*. (1998). Field measurements of crop height H_c (cm) were conducted in the field biweekly to define the uncertainty on the parameter presented in the literature. A similar range on the uncertainty of the other crop parameters is necessary to set up the model, i.e. Leaf Area Index LAI (-) and Root depth R_d (cm), were fixed on the basis of this variability. Direct soil samples were also sampled in the field at different depths, for analysis of the soil texture and bulk density. Then Pedotransfer Functions (PTFs) were used for the estimation of the soil hydraulic parameters in the model. In particular, considering the ranges of the soil texture in the field, a homogeneous soil profile was considered and PTFs of Zacharias & Wessolek (2007) and PTFs of Rawls & Brakensiek (1989) were applied for the estimation of the parameters of the soil retention curve and for the estimation of the hydraulic conductivity K_{sat} (cm/d), respectively. The uncertainty of each parameter was then fixed by considering a range in the parameters estimated as proposed by the authors of the PTFs. At the experimental site, the groundwater level is ~5 m below the surface as suggested by information from the State Environmental Agency based on a groundwater well nearby. The interaction between root zone and groundwater can be neglected and free drainage was set as the bottom boundary condition without introducing an error. Finally a warm-up period was used to eliminate the sensitivity to the initial conditions. Table 1 shows nominal values and ranges of uncertainty introduced for each of the input data and parameters.

Table 1 Ranges of uncertainty defined for the input factors. Weather data: random error introduced in the time series; Crop parameters: mean and random error introduced at maximum stage; Soil: mean and random error of parameters of Van Genuchten eq. (θ_r and L were fixed to 0.05 (–) and 0.5, respectively).

	Parameter	Range		Parameter	Mean	CV
Daily weather data (W)	Air Temperature (°C)	± 1.0	Crop parameters (C)	H_c max (cm)	130	8%
	Air humidiy (hPa)	± 0.2		R_d max (cm)	40	8%
	Wind (m/s)	± 1.0		LAI max (–)	2.5	8%
	Glob.Radiation (W/m^2)	± 20				
	Rain (mm)	± 2.0	Soil parameters (S)	θ_s (–)	0.38	5%
				n (–)	1.26	1%
				α (cm^{-1})	0.08	12%
				K_{sat} (cm/d)	200	40%

Codes and model set up

The study is conducted via SWAP model, a widely used 1D physically-based hydrological model of soil moisture dynamics in unsaturated soils based on the Penman-Monteith and Richards' equations (Kroes & Van Dam, 2003). In this study the uncertainty in the model structure is not explicitly considered comparing, for instance, models of different complexity (e.g. Baroni *et al*., 2010). However, the framework is applied with the final goal to optimize the monitoring activities and increase the model performance for groundwater recharge estimation.

Considering the monitoring activities described above, the sources of uncertainty were grouped in three main classes: meteorological data (W), crop parameters (C) and hydraulic soil parameters (S). Taking into account the range of uncertainty defined for each of the sources, a number of realizations n_i were defined, which cover the space of variability introduced. In particular, 64 realizations of meteorological data were created, 64 realizations of daily series of crop parameters were considered (i.e. LAI, H_c and R_d) and 64 realizations of hydraulic soil properties were generated. The realizations were sampled from the range defined in Table 1 and considering the correlation between parameters as detected in the measurements.

The simulations were run using a sampling number $N = 512$. In concordance to the methods proposed in Saltelli (2002), a total number of runs $N_R = N\,(k+2) = 2560$ was carried out, where $k = 3$ is the number of input factors (i.e. W, S, C). MatLAB codes were developed *ad hoc* with the SimLAB library (SimLAB, 2009) to run the Monte Carlo analysis and calculate the sensitivity indexes.

RESULTS

Uncertainty and sensitivity analysis of soil moisture

The results of the simulation of the mean soil moisture of the root zone (50 cm) in comparison with the measurements collected in the field (MR2) show a general agreement also without a specific model calibration (Fig. 1) underlining the good capability of the model to simulate the process. However, in the first period, when soil is relatively dry due to the high evapotranspiration rate (results not shown) and the low precipitation, the model tends to overestimates the process. In contrast, after intensive precipitation events (from DoY ~210), the model tends to underestimate the soil moisture measurements.

As expected, the sensitivity analysis shows that the soil properties (S) play a major role in the variability of the simulation results. Thus, these parameters are of higher importance for calibrating or improving the model performance in the simulation of the soil moisture dynamics.

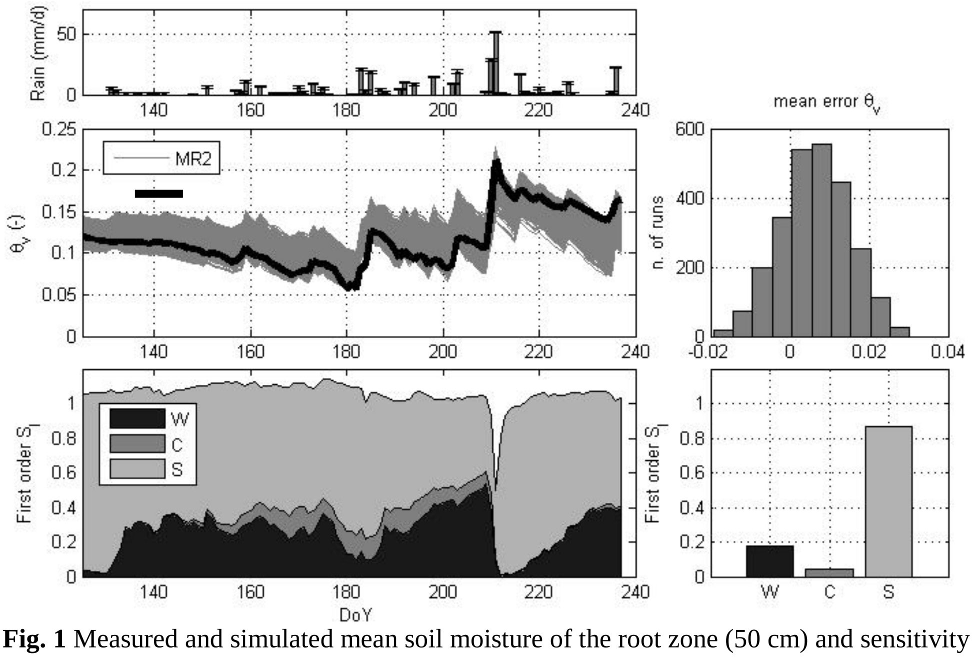

Fig. 1 Measured and simulated mean soil moisture of the root zone (50 cm) and sensitivity indexes.

However, if we look in more detail, the sensitivity analysis at daily time steps, the relative importance of the uncertainty of the weather data (W) and crop parameters (C) also become more important in relation to crop growth in particular for dry conditions. Finally, no particular differences are detected between First and Total sensitivity indexes, except during the highest precipitation event (DoY = 210) underlying a general independence of the input factors (results now shown).

Uncertainty and sensitivity analysis of evapotranspiration and groundwater recharge

Figure 2 shows the histograms of the cumulative evapotranspiration (ET_a) and of the groundwater recharge (Q_{bot}) below the root zone (50 cm) with the related sensitivity indexes. In these results, the uncertainty in the estimation of the evapotranspiration is relatively low, with mean value and range of ~270 and ±30 mm, respectively. However, the bottom fluxes are quite limited in the period considered, but the relative error becomes more important with mean value and range of ~25 ±30 mm, respectively. For both processes the ranges are comparable, suggesting that the errors in the model simulation can compensate each other and cannot be captured by the mean soil moisture. Moreover, it is important to notice that the range of uncertainty is much higher than the error introduced in the precipitation for the same period considered (i.e. ±6 mm, May–August). Further, it is interesting to see that soil properties (S) for these processes are not important sources of uncertainty, i.e. first sensitivity index is almost zero. This means that a better calibration of the soil properties will not improve the performance of the simulation of these processes, while for this goal reduction of sources of uncertainty has to be done to the weather condition (W) and of the crop parameters (C), respectively. Finally, differences between first and total indexes are detected for the groundwater recharge underlining the interaction between the input factors.

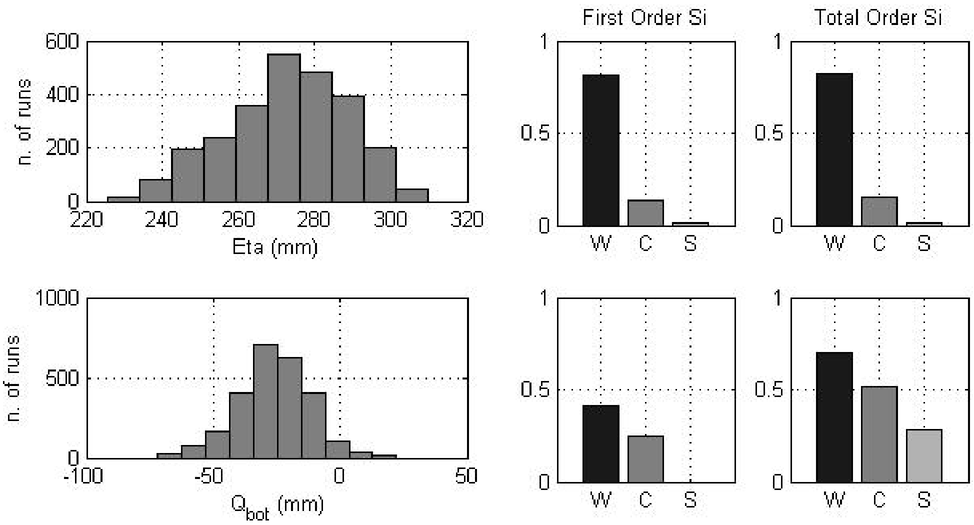

Fig. 2 Histograms of the cumulative values of the evapotranspiration (ET_a) and vertical flux of water below 50 cm, indicative for potential groundwater recharge (Q_{bot}). Both simulated by the model in the period considered. On the right sensitivity indexes are plotted.

In order to analyse in more detail the uncertainty of groundwater recharge, the results of the water fluxes at different depths are also compared (Fig. 3). Due to the relatively low precipitation rate in the period considered, the water fluxes already become negligible at a depth of 150 cm. However, the analysis can be easily extended in other cases characterized by deeper percolation and it is presented here as an example. From these results it is evident that the uncertainty related to the weather data (W) plays a major role in the uncertainty on the process also considered at a depth of 1.0 m. However, the relative importance of the soil parameters (S) tends to increase in opposition to the crop parameters (C). In such a way, with this analysis it is possible to understand at which depth the relative importance of the uncertainty in the upper boundary condition (W and C) becomes negligible. However, this could be analysed in more detail considering a longer monitoring period.

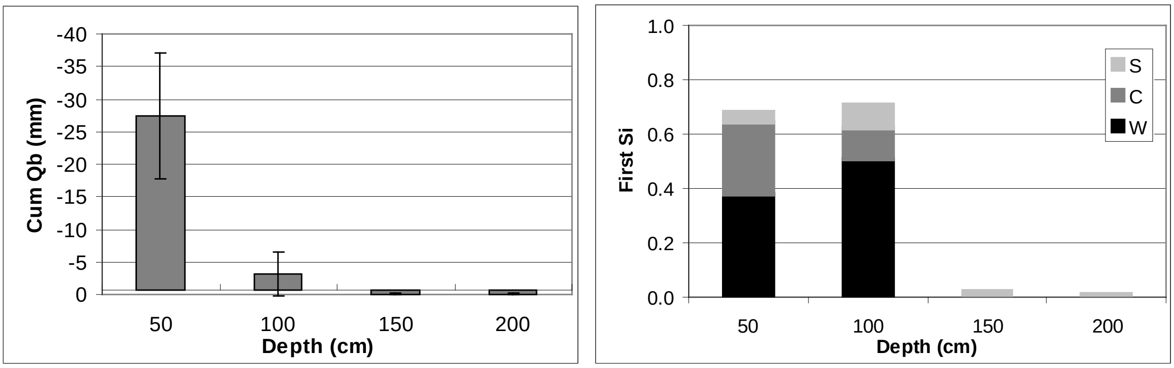

Fig. 3 Cumulative simulated vertical water flow indicative for potential groundwater recharge (Qbot), evaluated at different depths and related first sensitivity indexes. In the first diagram mean and standard deviation are shown.

CONCLUSIONS

The probabilistic framework used in this study is a useful approach for a global assessment of model performance and to identify the major sources of related uncertainty. Such information can be useful for purposes of model improvement, parameter estimation, or model simplification. This approach can in fact be used in a loop in order to optimize further activities that could improve the performance of the output considered. It can handle all the sources of uncertainty e.g. for input, distributed parameters or models structure and it can be easily implemented.

In the specific analysis, the framework was used for the assessment of groundwater recharge using the Richards-based hydrological model SWAP. The main conclusions are summarized as follows:

– Soil moisture pattern is quite well simulated by the model, but with a tendency to overestimate it during dry conditions and underestimate during wet conditions.
– Improvement in the simulation of the soil moisture could be done as expected by calibration of soil properties (S). These parameters have in fact the highest sensitivity index. Anyway the analysis at daily time steps also underlines that the relative importance of the other factors changes in time.
– Evapotranspiration and the bottom flux at 50 cm depth simulated by the model show an uncertainty of the same order of magnitude i.e. ±30 mm. These errors can compensate each other and cannot be captured by the error in the simulation of the mean soil moisture.
– The major sources of uncertainty related to the estimation of evapotranspiration and of vertical water fluxes at 50 cm and 100 cm are the weather data (W) and the crop parameters (C). Thus, an improvement of the model by calibrating the soil properties will not reduce the uncertainty in these outputs. However, an improvement can be achieved by focusing the further activities in the reduction of the uncertainty at the upper boundary condition, e.g. installing a new meteorological station close to the experimental site or improving the extrapolation of the existing weather data.
– Due to the low precipitation rate in the monitoring period, the bottom fluxes were negligible already at the depth of 150 cm. However, the analysis shows an example of how to define at which depth the uncertainty in the upper boundary condition could become less important in comparison with the definition of the soil parameters. Further analysis will be conducted by

considering a longer monitoring period in order to analyse the relative importance also when deeper percolation is considered that should result in actual groundwater recharge.

– Finally, a finer analysis with this probabilistic framework can treat each set of soil parameters, crop parameters or weather data separately, allowing determination of which one could be more important. This was not the goal of the present study but it could be an important issue in further research.

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