QUICS: Quantifying Uncertainty in Integrated Catchment Studies

D4.1 Report on strategy to investigate the entire model uncertainty chain in rural landscapes so as to provide probabilistic outputs to urban modelling end-users

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Acronyms and Abbreviations

a.s.l	Above sea level
ABC	Artificial Bee Colony
DEM	Digital Elevation Model
Dream	DiffeRential Evolution Adaptive Metropolis Algorithm
FAST	Fourier Amplitude Sensitivity Test
FSCABC	Fitness Scaled Chaotic Artificial Bee Colony
GLUE	Generalized Likelihood Uncertainty Estimation
HRU	Hydrological Response Unit
JLU	Justus Liebig University Giessen
LHS	Latin Hypercube Sampling
LULC	Land Use/Land Cover
MLE	Maximum Likelihood Estimation
MCMC	Markov-Chain Monte Carlo
MPI	Messaging Passing Interface
NSE	Nash–Sutcliffe Efficiency
ROPE	RObust Parameter Estimation
SA	Simulated Annealing
SCE-EA	Scuffled Complex Evolution Algorithm
SPOTPY	SPOTting Model Parameters Using a Ready-Made Python Package
SWAT	Soil and Water Assessment Tool
95PPU	95% prediction uncertainty

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Executive Summary

This deliverable describes a strategy for model calibration and uncertainty assessment, which has been developed and is currently being tested using data obtained from the Schwingbach Earth Observatory located in the Federal State of Hesse in Germany. This observatory is located in a low mountain area, with the 3.7 km^2 catchment containing a human impact landscape containing channelized streams, piped drainage networks, combined sewer overflows and fish ponds. The strategy is demonstrated using a parameter rich model, called SWAT combined with the SPOTPY computational tool which is used to estimate the level of parameter uncertainty. The strategy has a 3 stages: (1) problem definition, (2) model calibration, (3) results analysis. A SWAT model for the catchment was built. This model was linked to the automated parameter estimation and uncertainty analysis package SPOTPY using a Python interface. This interface was used to calibrate the model using the principles of GLUE and the logarithm of the NSE was used as the objective function. The level of parameter uncertainty was estimated using the extremes of the parameter distributions. The calibrated SWAT model was able to simulate the low flows well but struggled with the higher flow conditions.

Further work is continuing considering different parameter sampling strategies and looking in more depth on the uncertainty created by highly spatially variable rainfall that this catchment is thought to experience. Different parameter estimation and objective functions will also be studied to examine their impact on the estimation of the level of parameter uncertainty.

CONTENTS

1 Background

As part of the deliverables in the QUICS project, the project partner from Justus Liebig University Giessen (JLU) first developed a software package to estimate the uncertainty of various hydrological model components (see Deliverable 1.4). The platform free and independent software package SPOTPY (Houska et al., 2015) was used to parameterize the Soil and Water Assessment Tool (SWAT). In a first set up, we investigated the effect of input data uncertainty on model outputs for a rural catchment in Luxemburg (Camargos et al., 2018). We analyze eight different setups for SWAT, i.e. different setups regarding the land-use, elevation, and soil input data. We showed that despite presenting similar parameter uncertainty for all setups, the results followed a disparate parameter posterior distribution. This indicates that at least part of the model uncertainty is compensated by the fitted parameter values.

In a next step, we are therefore interested in the uncertainty chain of hydrological modelling, which is introduced by a variety of decisions that need to be taken and the data that can be used when simulating water or nutrient fluxes in complex catchments using parameter intensive models such as SWAT. As part of this Deliverable 4.1, we present a strategy for model calibration and uncertainty assessment, which has been developed and is currently tested in the Schwingbach Earth Observatory, Federal State of Hesse, Germany.

2 Study area

The study site is part of the Schwingbach catchment, an area of a low mountainous creek (Vollnkirchener Bach) in the municipality of Hüttenberg, Hesse, Germany (50◦2905600 N, 8◦330200 E). The landscape is anthropogenic-influenced having the physical structure of the stream system altered: channeled stream reaches, drainage systems/pipes, combined sewer overflows, and fishponds. The area is part of the Schwingbach Earth Observatory of the Justus Liebig University Giessen (Orlowski et al., 2014), see Figure 1.

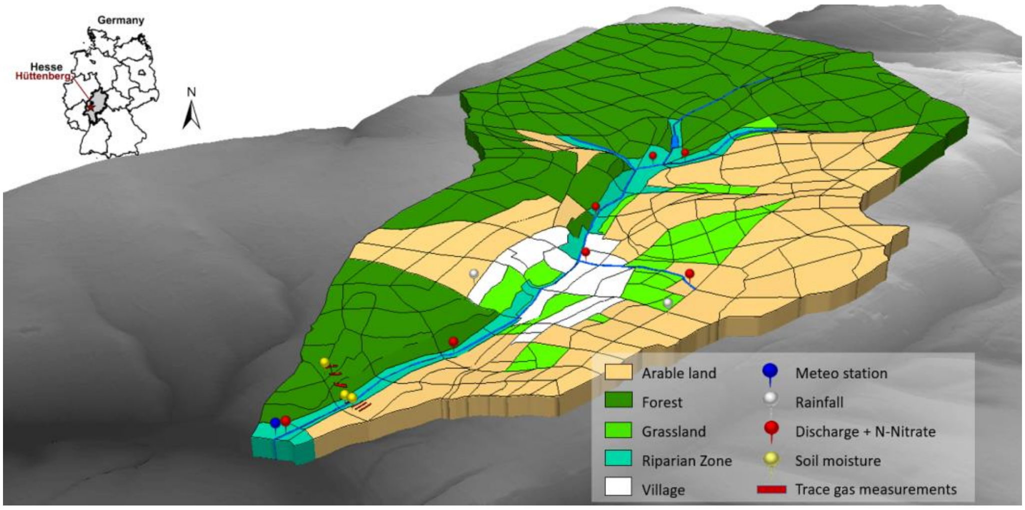

Figure 1: Digital elevation model and land use of the Vollnkirchener Bach catchment. The map shows available sampling sites and types of measurement data. Continuous high-resolution data measurements for discharge and nitrate instream are available at the catchment outlet and are used as validation data in this study.

Soils are agricultural *Stagnosols* with thick loess layers (*Stagnic Luvisols*) as well as forested *Cambisols*, and also *Gleysols* under grassland sites along the streams. The land use is dominated by forest and arable land, presenting areas with grassland along the stream and a small portion of urban settlement. Elevation ranges from 235 to 351 m a.s.l. The climate is classified as temperate, with a mean annual precipitation of 588 mm, and a mean annual temperature of 10.5 ◦C for the hydrological year 1 November 2013–31 October 2014 (Seifert et al., 2016).

3 Concept used to investigate the model uncertainty chain

We followed three main steps to estimate the model uncertainty chain, which are summarized in Figure 2 and explained in details in the following text.

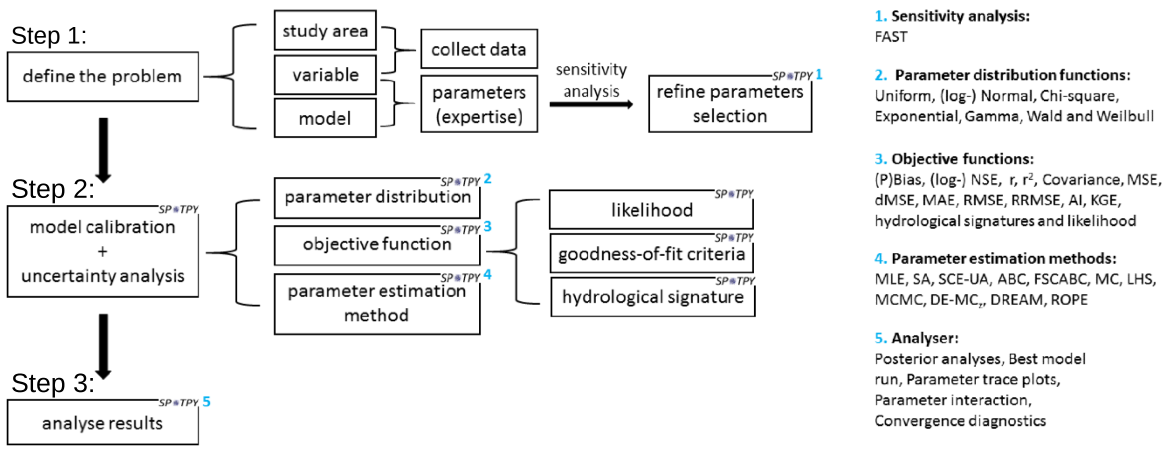

Figure 2: Calibration and uncertainty analysis three-step process. The superscripted numbers indicate the technical methods applied with the SPOTPY package (Houska et al. 2015).

<u>Step 1:</u> SWAT is a semi-distributed model that requires a diversity of specific information as input data. The basic information are related to topography, soil properties, vegetation, and meteorology. A digital elevation model (DEM) is used to delineate the watershed, estimate the stream network and slope. After uploading the DEM map to the ArcSWAT interface (ArcSWAT 2012 version), the user has the option of defining how detailed the drainage network will be by selecting the upstream drainage area value. We set this value to the minimum recommended by the ArcSWAT interface. We considered all outlets automatically generated by the interface as valid and defined the location where the water quantity and quality data were collected as the main outlet of the catchment. As a test case for this deliverable, we used data from the Schwingbach Earth Observatory, Federal State of Hesse, Germany. This watershed has an overall area of 3.7 km² and is partitioned into several sub-basins based on the location of each outlet. The hydrologic response unit (HRU) is the smallest component of a SWAT watershed in SWAT. An HRU is defined as a land area comprised of a unique combination of land use/land cover (LULC), soil, and slope class information. We included a soil map containing three different soil classes, and

a LULC map identifying areas covered by forest, pasture, agriculture, water and urban settlement. Further, we defined three slope classes, i.e. <7%, 7-15% and 15%, which are considered as moderate, medium and steep slopes. Further, we used land management information from a local farmer to define the crop rotation during the simulated period. We included daily weather data as forcing data. Minimum and maximum temperatures, relative humidity, wind speed, solar radiation, and precipitation were collected from a station 1 km north-west of the study area. Additionally, two other stations inside the study area were considered to cover the spatial variability of the precipitation information. Daily evapotranspiration rates were estimated by the Hargreaves method.

<u>Step 2</u>: In order to connect SWAT with SPOTPY, we developed a universal Python-SWAT interface (Camargos et al., 2018). The interface comes along with a parameter writing routine, which takes the parameter names and their value and automatically writes them into the corresponding SWAT input files. SWAT is then started from Python and the results can be read with a self-developed SWAT_readout library, which returns the simulated discharge. The comparison of observed data and the assignment of an objective function value to each run is done with SPOTPY. The whole process is automatized and can be started in parallel by using a Message Passing Interface (MPI).

With this set up, we calibrated SWAT with daily discharge from the main watershed outlet, a gauging station equipped with a continuous water level sensor and an RBC-flume to convert water levels into discharge. We selected a large (n=18) parameter group to be considered in the calibration of SWAT based on expert-knowledge and experience obtained in the the previous Luxemburg study. Afterward, we run the Fourier Amplitude Sensitivity Test (FAST) to refine the number of parameters to the 10 most sensitive ones for discharge simulations (Figure 2, Step 1/1). For the model calibration and parameter uncertainty analysis, we used the principle of the Generalized Likelihood Uncertainty Estimation (GLUE) methodology. We assumed a non-informative uniform prior distribution for the parameters (Figure 2, Step 2/2). We assessed model performance by the Nash–Sutcliffe Efficiency (NSE) (Figure 2, Step 1/3). As the squared residuals of the NSE calculation overemphasize high values, we also considered the logarithmic NSE (log NSE), which is more sensitive to low flows. We sorted the results by descending order of NSE and log NSE and considered the 5% top as the remaining posterior distribution. The parameter space was investigated by Latin Hypercube Sampling (LHS) with 1,000 repetitions (Figure 2, Step 2/4). All required decisions and calculation in Step 2 were performed using the SPOTPY tool developed in our group as part of Deliverable 1.4 (Houska et al. 2015).

<u>Step 3:</u> The parameter uncertainty is then estimated using the measured P- and R-factors (Figure 3, Step 3/5). The P-factor is the percentage of data bracket by the 95% prediction uncertainty (95PPU) which is calculated at the 2.5 and 97.5 percentiles of the simulated data. The R-factor is the ratio of the average distance between the upper and lower 95PPU and the standard deviation of the measured data. Ideally, the P-factor tends to 1 and the R-factor is close to 0.

As first results, we show that SWAT is capable to reproduce the flow dynamics and the overall water balance of the research catchment Vollnkirchener Bach. Figure 3 indicates that the SWAT model is simulating low flows properly. However, the low performance regarding the NSE values, ranging from 0.28 to 0.40, indicates that the current SWAT set up cannot estimate the high flow peaks.

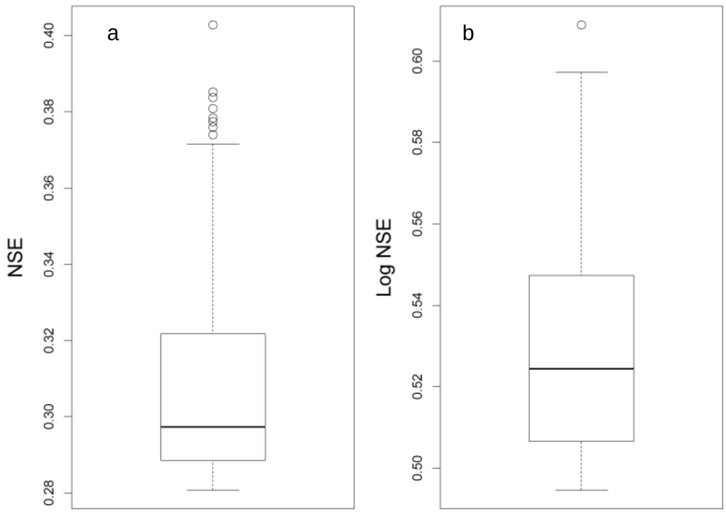

Figure 3: Posterior SWAT performance evaluated for different goodness-of-fit criteria: a) NSE and b) log NSE.

A closer look at the timing and height of the simulated versus the observed hydrograph reflects errors depicted in Figure 4. We identified two major problems:

1) The model needs a warm up period of about 6 months for the time between January to June 2013 (Figure 4). We will implement this in the ongoing investigation.

2) Some of the remaining errors in the fit of the observed high flows may be explained by the geographical location of the rainfall stations that are outside of the study area. From field reconnaissance trips and reports from local people, we know that precipitation is highly variable in space. To overcome this limitation, the next step will be to implement a methodology to account for rainfall uncertainty during the calibration and validation procedure (Kavetski et al., 2006).

As work in Step 3 is still in progress, we will consider further parameter sampling strategies apart from the aforementioned Latin Hypercube Sampling. For the next couple of months, the SWAT model set up will be used to investigate the effect of selecting different objective functions (likelihoods that allow the assessment of measured data uncertainty) (Figure 4, Step 2/3) and different parameter estimation methods, such as the Markov-Chain Monte Carlo (MCMC) sampler and the Scuffled Complex Evolution Algorithm (SCE-UA) (Figure 1, Step 2/4).

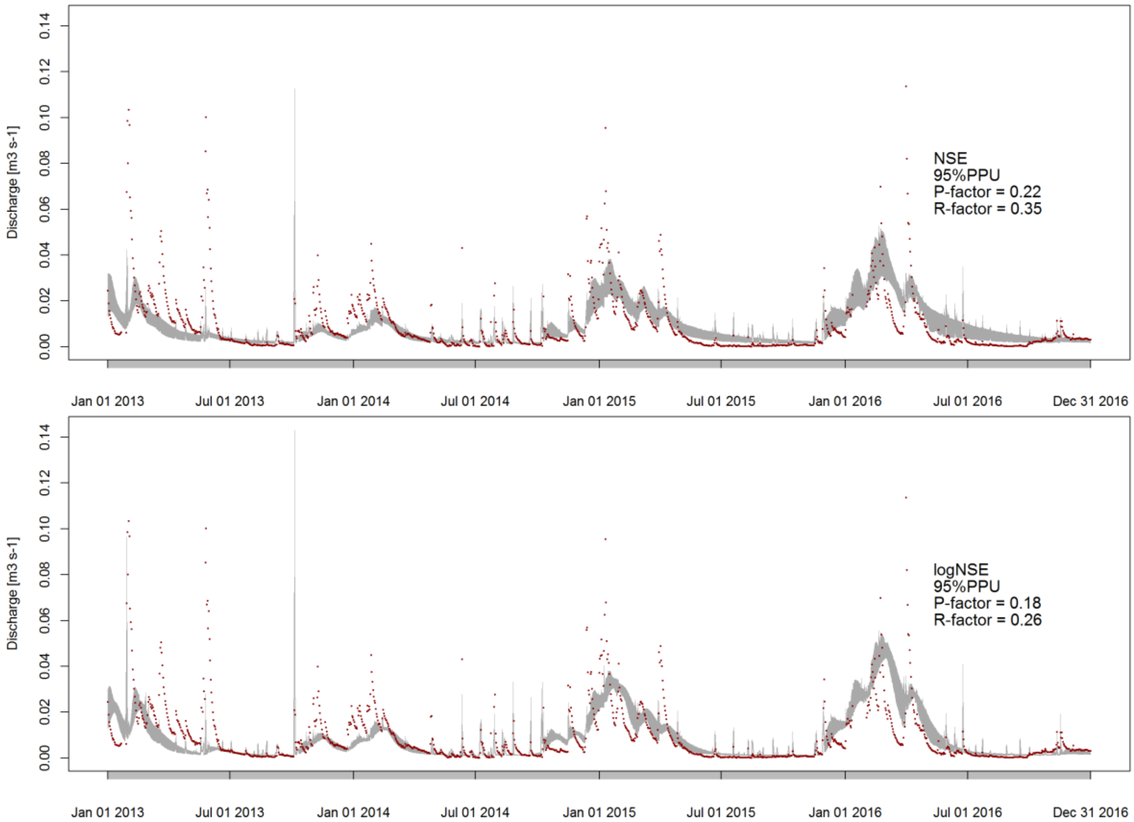

Figure 4: Hydrographs comparing the posterior model results for different goodness-of-fit criteria. The plots include the 95% prediction uncertainty, and the P- and R- factors.

4 Outlook

Complex formal Bayesian, informal Bayesian and non-Bayesian algorithms bring complex tasks to link them with a given model. SPOTPY makes this task as easy as possible. Some features one can use within the SPOTPY package and which will be considered in future work of SWAT applications in the Schwingbach Earth Observatory and elsewhere are:

- **Fitting models** to evaluate data with different algorithms. Available algorithms are Monte Carlo (MC), Markov-Chain Monte-Carlo (MCMC), Maximum Likelihood Estimation (MLE), Latin-Hypercube Sampling (LHS), Simulated Annealing (SA), Shuffled Complex Evolution Algorithm (SCE-UA), DiffeRential Evolution Adaptive Metropolis Algorithm (Dream), RObust Parameter Estimation (ROPE), Artificial Bee Colony (ABC), Fitness Scaled Chaotic Artificial Bee Colony (FSCABC) and Fourier Amplitude Sensitivity Test (FAST).
- Wide range of **objective functions**, likelihood functions and hydrological signatures to validate the sampled results. Available objective functions are: Bias, Nash-Sutcliff (NSE), log Nash-Sutcliff (logNSE), Logarithmic probability (logp), Correlation Coefficient (r), Coefficient of Determination (r^2), Mean Squared Error (MSE), Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), Relative Root Mean Squared Error (RRMSE), Agreement Index (AI), Covariance, Decomposed MSE (dMSE) and Kling-Gupta Efficiency (KGE).

- Wide range of **likelihood functions** to validate the sampled results: logLikelihood, Gaussian Likelihood to account for Measurement Errors, Gaussian Likelihood to account for Heteroscedasticity, Likelihood to account for Autocorrelation, Generalized Likelihood Function, Laplacian Likelihood, Skewed Student Likelihood assuming homoscedasticity, Skewed Student Likelihood assuming heteroscedasticity, Skewed Student Likelihood assuming heteroscedasticity and Autocorrelation, Noisy ABC Gaussian Likelihood, ABC Boxcar Likelihood, Limits Of Acceptability, Inverse Error Variance, Shaping Factor, Nash Sutcliffe Efficiency Shaping Factor, Exponential Transform Shaping Factor, Sum of Absolute Error Residuals.
- Wide range of **hydrological signature functions** to validate the sampled results: Slope, Flooding/Drought events, Flood/Drought frequency, Flood/Drought duration, Flood/Drought, variance, Mean flow, Median flow, Skewness, compare percentiles of discharge.
- Prebuild **parameter distribution functions**: Uniform, Normal, lognormal, Chi-square, Exponential, Gamma, Wald, Weilbull.
- SPOTPY is platform independent and due to the MPI support it can make use of fast parallel computing.

5 References

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