Using discharge data to reduce structural deficits in a hydrological model with a Bayesian inference approach and the implications for the prediction of critical source areas

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[1] A distributed hydrological model was used to simulate the distribution of fast runoff formation as a proxy for critical source areas for herbicide pollution in a small agricultural catchment in Switzerland. We tested to what degree predictions based on prior knowledge without local measurements could be improved upon relying on observed discharge. This learning process consisted of five steps: For the prior prediction (step 1), knowledge of the model parameters was coarse and predictions were fairly uncertain. In the second step, discharge data were used to update the prior parameter distribution. Effects of uncertainty in input data and model structure were accounted for by an autoregressive error model. This step decreased the width of the marginal distributions of parameters describing the lower boundary (percolation rates) but hardly affected soil hydraulic parameters. Residual analysis (step 3) revealed model structure deficits. We modified the model, and in the subsequent Bayesian updating (step 4) the widths of the posterior marginal distributions were reduced for most parameters compared to those of the prior. This incremental procedure led to a strong reduction in the uncertainty of the spatial prediction. Thus, despite only using spatially integrated data (discharge), the spatially distributed effect of the improved model structure can be expected to improve the spatially distributed predictions also. The fifth step consisted of a test with independent spatial data on herbicide losses and revealed ambiguous results. The comparison depended critically on the ratio of event to preevent water that was discharged. This ratio cannot be estimated from hydrological data only. The results demonstrate that the value of local data is strongly dependent on a correct model structure. An iterative procedure of Bayesian updating, model testing, and model modification is suggested.


1. Introduction

[2] The contamination of water bodies with agrochemicals is of environmental concern and effective mitigation strategies are needed [Reichenberger et al., 2007]. Such strategies rely on an accurate understanding and quantification of the relevant fate and transport processes. Our approach was to focus on the spatial distribution of areas contributing to diffuse pollution of surface waters by agrochemicals. It has been demonstrated that the distribution of these areas is strongly related to hydrological conditions, especially to the occurrence of fast flow processes, primarily surface runoff and macropore flow to tile drains [e.g., Pionke et al., 2000; Leu et al., 2004b; Heathwaite et al., 2005]. If such areas coincide with locations where nutrients or pesticides are available for transport, they are called critical source areas (CSA). The delineation of CSA is a prerequisite for effective mitigation of surface water contamination.

[3] The use of spatially distributed hydrological models is mandatory to obtain a spatially differentiated model response [e.g., Quinn and Beven, 1993; Frankenberger et al., 1999]. Such models require spatially differentiated input data for their implementation. Except for digital elevation models (DEM), spatial data are in general neither easily available nor measurable at an appropriate resolution. For practical applications, model input has to be estimated from generally available data like soil maps or land use data, which are often coarse and lead to rather large uncertainties in model predictions. However, one has not only to account for uncertainty in the model parameters but has to address uncertainties in the model structure, in external input factors, or even in the numerical solution [Beck, 1991]. Uncertainties in hydrological models have been discussed intensively, but until now no generally accepted method to address all the different sources of uncertainty has been established (see discussion by Mantovan and Todini [2006] and Beven et al. [2008]). Classes of techniques that...
have been suggested for model calibration and uncertainty estimation include classical Bayesian [e.g., Kuczera and Parent, 1998; Bates and Campbell, 2001; Vrugt et al., 2003a; Kavetski et al., 2006a; Huard and Mailhot, 2008], pseudo-Bayesian (e.g., GLUE, introduced by Beven and Binley [1992]), multiple-criteria approaches [Gupta et al., 1998; Vrugt et al., 2003b], and Bayesian model averaging [Vrugt and Robinson, 2007].

For a practical implementation of mitigation and management strategies, it is crucial to reduce the uncertainties as much as possible and to correctly communicate the uncertainties to stakeholders. An obvious way to reduce uncertainty is to search for additional information which has not been used to formulate and parameterize the model. In many cases, discharge data is available. It has the advantage of integrating processes in the entire catchment but it does not provide spatially resolved information (unless multiple gauging stations are used [e.g., Anderson and Burt, 1978]). Since mechanistic hydrological models typically have many spatially distributed parameters, the achievable reduction in parameter uncertainty through discharge data may be limited. In order to examine to what extent this is the case, we combined prior information on soil properties derived from the spatial distribution of soil types and texture with measured discharge data by Bayesian inference.

In Bayesian statistics, probability distributions are used to describe the knowledge or belief of individuals. When applying these techniques in environmental decision support, it is the analyst’s objective to obtain defensible, intersubjective current scientific knowledge [Gillies, 1991], rather than the subjective belief of an individual scientist. Prior knowledge about the model structure is described by the likelihood function of the model. Prior knowledge about model parameter values is described by the prior probability distribution of the parameters. This prior information is then combined with observed data using the theorem of Bayes to derive the posterior (updated) probability distribution of model parameters and results [Gelman et al., 2004; O’Hagan, 2003]. The updating procedure is usually implemented by a Markov chain Monte Carlo (MCMC) algorithm. This has previously been done with hydrological models [e.g., Kavetski et al., 2006b; Yang et al., 2007; Huard and Mailhot, 2008]. However, because of poor identifiability there may still be a relatively large volume in parameter space that contains parameters leading to similarly good results. In a Bayesian context, this is reflected by a posterior that is flat in certain directions in parameter space.

To account for different sources of uncertainty, an adequate error model is required. As frequentist probabilities follow the same mathematical rules as Bayesian probabilities, and the frequentist interpretation is a natural defensible, intersubjective belief about the outcome of random processes, we can combine a frequentist likelihood function of a system that contains random elements with Bayesian priors. Because of memory effects in the model, the effect of (random) input errors and errors in the model structure lead to autocorrelated errors in model output. Despite updating our knowledge of model parameters in a Bayesian framework, we are then able to apply frequentist tests to the residuals at the maximum of the posterior (as the best guess for the “true” parameter values) to check the statistical assumptions formulated by the likelihood function. Note, however, that we cannot apply frequentist tests to our posterior model predictions as their uncertainty combines frequentist uncertainty of the likelihood function (for given parameter values) with uncertain knowledge formulated by the posterior parameter distribution.

We carried out our investigations in a small agricultural catchment in Switzerland. The simulations were done with the spatially distributed water balance model SMDR (soil moisture distribution and routing model) [Soil and Water Laboratory, 2003], which has been used for delineating CSAs in small agricultural catchments of the eastern United States [e.g., de Alwis et al., 2007; Frankenberger et al., 1999; Gerard-Marchant et al., 2006], Frey et al. [2009] showed, on the basis of a priori estimated parameters, that the simulated discharge in our study catchment agreed with the measured data but the prediction carried a large uncertainty. The predicted spatial distribution of fast transport processes matched the observed herbicide losses from three different subcatchments very closely. Consideration of connectivity of surface flow was crucial to obtain this result.

The objective of this work was to analyze the uncertainty in CSA prediction that is solely based on data generally available to land managers (soil maps, land use, topography) and to determine to what degree it can be reduced using river discharge data within a particular case study. First, we quantified the uncertainty of the prior prediction described by Frey et al. [2009]. Therefore, the best guess model parameters were extended to prior probability distributions and propagated through the deterministic model. This was implemented numerically by Monte Carlo simulation. The second objective consisted of investigating to what degree the prediction uncertainty can be reduced by using measured discharge to constrain the model parameters. Therefore, it was necessary to carefully formulate a likelihood function of the model and to test its statistical assumptions. As this led to the identification of deficits in the model structure, we improved the model in a third step to reduce systematic errors. Finally, we investigated how the three different levels of modeling (prior, calibrated original and calibrated improved model) affected the spatial prediction of saturated areas in the catchment and how these spatial predictions agree with observed herbicide losses at the level of three subcatchments.

2. Methods

2.1. Study Area and Calibration Data

The study site is a small agricultural catchment of 1.9 km² within the Swiss plateau (Figure 1). It has a moderate topography (average slope of 3.4%), the elevation ranges from 490 to 550 m above sea level, and the annual precipitation averages 1330 mm. The elevation and the soil map of the catchment are shown in Figure 2. Details are given by Leu et al. [2004a] and Frey et al. [2009].

During three growing seasons, herbicide losses in different parts of the catchment were monitored. We focused on a controlled herbicide application in the year 2000 [Leu et al., 2004a, 2004b]. All corn fields in the catchment, but not any other field, were treated with the same herbicide mixture (including atrazine, dimethenamid, and metolachlor) on the same day. In the weeks following the
application (5 May to 1 August) discharge and herbicide concentrations were measured in the stream at the outlets of three subcatchments (Figure 1). Furthermore, two weather stations in the catchment recorded precipitation and air temperature. We used this data for model calibration and validation (see section 3.6).

2.2. Original Model

[11] To describe the hydrological processes in the catchment we used a slightly modified version of the SMDR model [Frey et al., 2009]. This is a spatially distributed hydrological water balance model designed to predict saturated areas which contribute to surface runoff. The code of SMDR is implemented in the GIS environment GRASS (http://www.grass.itc.it). The model is shortly described in the following paragraphs; details can be found in the manual [Soil and Water Laboratory, 2003].

[12] The catchment is divided into uniform squares (soil columns) with multiple layers (Figure 3). The model is driven by precipitation as primary model input. If the area is not sealed, all water infiltrates into the top layer, else the water is treated as surface runoff. The lateral and vertical water flow between model cells is calculated on the basis of a simplified version of Darcy’s law (gravity flow). For lateral flow, the hydraulic gradient is calculated differently depending on the presence of artificial subsurface drains. Without drains the gradient is assumed to be equal to the local slope (kinematic wave approximation [e.g., Beven, 1981]) with a minimum gradient in flat areas. If a soil is artificially drained the hydraulic gradient is approximated by a mean hydraulic gradient (drainage efficiency coefficient $E_d$). The hydraulic conductivity is described by an exponential dependence on the water content. Above a certain threshold level of water content, macropore flow is considered and estimated by multiplying the hydraulic conductivity with a model parameter $\tilde{C}_20$, which exponentially decreases with depth. Lateral water routing in the soil to downslope neighboring cells of the same layer is based on the $D_\infty$ algorithm of Tarboton [1997]. This algorithm distributes outflow depending on the cell slope aspect.

[13] Evapotranspiration is calculated on the basis of the daily potential evapotranspiration provided by MeteoSchweiz, the growth of the vegetation and the actual soil

Figure 1. Aerial picture of the study catchment with its three subcatchments and its position within Switzerland. The corn fields of the study campaign in 2000 are framed by a brown line [Leu et al., 2004a]. Swissimage, vector25 © 2003, reproduced with the permission of swisstopo, JA082266.

Figure 2. (a) Elevation and (b) soil map of the catchment. The boundaries of the corn fields of the field study in 2000 are delineated, and the brook is shown (dotted line where it flows in a culvert).
In the improved model the constant, soil-type specific percolation rate (\(\text{per}_{\text{soil}}\)) that changes with the height of the water table, \(h\), by introducing a soil-specific factor \(f_{\text{soil}}\):

\[
\text{per}_{\text{soil}} = h f_{\text{soil}}.
\]  

(2)

In a similar way the gradients on drained areas were made dynamic by describing the drainage efficiency as a function of the water table. The gradient on drained areas is multiplied by the level of the water table, \(h\), and a lateral factor, \(f_{\text{lat}}\):

\[
\beta_{\text{drained}} = h f_{\text{lat}} \text{const}.
\]  

(3)

In addition, we accounted for the possibility that there is some exchange of groundwater across the catchment boundaries by introducing a parameter \(\gamma_{\text{ground}}\) that extracts or adds a constant fraction of the percolated water. The flow rate out of the soil column is then equal to \(\text{per}\), whereas the flow rate into the base flow reservoir is given by

\[
Q_{\text{in reservoir}} = \text{per} (1 - \gamma_{\text{ground}}).
\]  

(4)

Furthermore, since one run of the model lasted too long to obtain a sufficient number of simulations required for a statistical analysis, we had to rewrite the water balance calculation part of the modified model. This part was transferred from GRASS into a faster language (FORTRAN 95). We refer to this model as the “improved model.”

### 2.4. Prior Parameter Distribution

For parameterization, the SMDR model requires spatially distributed information about topography, land use, and soil parameters. This spatially distributed information has to be combined with parameters describing the properties of the different land use classes. In addition, some general parameters (such as drainage efficiency or macropore coefficients) are required.

On the basis of the prior knowledge (see below), it was possible to characterize most marginal prior distributions by upper and lower bounds, an average value and the

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**Figure 3.** Conceptual overview of the water fluxes considered in a soil column in the SMDR model.
vance. According to the Minimal Relative Entropy concept [Woodbury and Ulrych, 1993, 2000] this information results in (truncated) (log)normal distributions, which were assumed to be independent. Since prior information for general parameters and the percolation rates was vague, wide distributions were chosen (Tables 1 and 2). These parameters for the priors were derived from literature, other modeling studies, and expert knowledge as described by Frey et al. [2009]. For the soil type-specific percolation factors, the means (Table 2) were estimated from observed specific discharge data under base flow conditions. Thereby, it was assumed that they were the smaller the wetter the soil type. The variance was chosen such as to have a relatively flat distribution between 0 and 2 day^{-1}.

[23] The prior values of the hydrological parameters were calculated by pedotransfer functions [Schaap et al., 2001] from texture data extracted from the soil map. For the model the van Genuchten parameter saturation water content, \( \theta_{sat} \), the residual water content, \( \theta_{r} \), a measure of the pore size distribution, \( N \), the inverse air entry suction, \( \alpha \), and the saturated hydrological conductivity, \( K_{sat} \), were relevant [van Genuchten, 1980].

[24] In order to limit the number of soil hydraulic parameters and to maintain the spatial structure obtained from the soil map, the soil parameters were multiplied by factors specific to the various soil types and horizons (similar to rainfall multipliers by Kavetski et al. [2006a, 2006b] and Vrugt et al. [2008]). These multipliers were then used as model parameters instead of the original physical soil parameters, which were kept at their original values. The marginal prior distributions of the multipliers of each hydrological parameter were assumed to be equal for all soils (Table 3). Their expected values were equal to one and their coefficients of variation (CV) corresponded to the CV of the underlying quantity as estimated in the pedotransfer function. Some truncations of the distribution were necessary to assure that the parameters are in a reasonable range (e.g., that \( \theta_{sat} \) is larger than \( \theta_{r} \)). Nine soil types and three soil layers still led to 135 multipliers in total. To reduce the number of parameters, we considered only the most important soil types and horizons. These were identified on the basis of the local sensitivity analysis performed by Frey et al. [2009]. It would have been advantageous to perform a global sensitivity analysis instead [Saltelli et al., 2000]; but the computational cost of runs of the simulation program prevented an application of this technique. This is probably not a severe problem as we did not use the sensitivity coefficients for any quantitative analysis and only omitted parameters with a very low sensitivity. The sensitive parameters were those associated with the A horizon of the forest, Cambisols, Eutric-Gleysols, and Gleyssols, the B horizon of Cambisols, and the C horizon of Cambisols and forest. These parameters all relate to the dominant soils in the catchment. This confirms that the local sensitivity analysis may be a reasonable approximation to global sensitivities, at least with respect to the identification of sensitive parameters. The remaining parameters were fixed at their original values.

[25] According to Frey et al. [2009] river discharge was highly sensitive to meteorological inputs (precipitation and potential evapotranspiration rate). However, since rainfall was directly measured in the catchment and its spatial variability within the small catchment was relatively low, we assumed input uncertainty to be small and did not consider this type of uncertainty.

2.5. Uncertainty Analysis of Prior Prediction

[26] Frey et al. [2009] carried out a prior simulation with the parameter values labeled “mean” in Tables 1–3. We assessed the uncertainty in the a priori prediction by propagating the prior distribution through the deterministic simulation model. This was done by a Monte Carlo simulation of sample size 500 using UNCSIM, a computer program for statistical inference and sensitivity, identifiability and uncertainty analysis [Reichert, 2005, 2006].

2.6. Bayesian Inference

[27] In order to obtain information on how the parameter distribution changes when using additional data, we evaluated the posterior distribution of parameters given the data \( p(\theta|y^{obs}) \) using the theorem of Bayes [Gelman et al., 2004]:

\[
p(\theta|y^{obs}) = \frac{p(y^{obs}|\theta)p(\theta)}{\int p(y^{obs}|\theta')p(\theta')d\theta'},
\]

where \( p(\theta) \) is the prior probability density of parameters and \( p(y|\theta) \) is the likelihood function of the model, i.e., the probability density of model results, \( y \), given the parameters.

[28] The deterministic model is a function of model parameters, \( \theta \), and the structure of the deterministic part of

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Distribution</th>
<th>Mean</th>
<th>SD</th>
<th>Minimum</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drainage efficiency*</td>
<td>( E_d )</td>
<td>transformed normal( ^{f} )</td>
<td>28</td>
<td>10</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>Sink drain efficiency (%)</td>
<td>( M_{sink} )</td>
<td>normal</td>
<td>10</td>
<td>20</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>Conductivity multiplier for the macropore flow</td>
<td>( \kappa )</td>
<td>normal</td>
<td>10</td>
<td>10</td>
<td>1</td>
<td>100</td>
</tr>
<tr>
<td>Linear base flow coefficient (%)</td>
<td>( LBC )</td>
<td>normal</td>
<td>50</td>
<td>30</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>Deep percolation (%)</td>
<td>( \gamma_{ground} )</td>
<td>normal</td>
<td>0</td>
<td>1</td>
<td>-5</td>
<td>100</td>
</tr>
<tr>
<td>Lateral drainage gradient (%)</td>
<td>( f_{lat} )</td>
<td>normal</td>
<td>1</td>
<td>3</td>
<td>0</td>
<td>1000</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>( \sigma )</td>
<td>inverse</td>
<td>1</td>
<td>1000</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*The normal and lognormal distributions are truncated at minimum and maximum. Mean and SD refer to the means and standard deviations of the non-truncated distributions.

Only investigated in the calibration of the original version.

Because of model constraints the sample for \( E_d \) was drawn from an underlying normal distribution of \( \mu_{E_d} = \frac{14}{25} \). It means, \( \mu_{E_d} \) and standard deviation, \( \sigma_{E_d} \), are given. The probability density of \( E_d \) is then given by \( f(E_d) = \frac{1}{\sigma_{E_d}\sqrt{2\pi}} \exp\left[ -\frac{1}{2} \left( \frac{E_d - \mu_{E_d}}{\sigma_{E_d}} \right)^2 \right] \).

Only investigated in the improved model structure.

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the model, $M$. The discrete output, corresponding to observations, can be represented by a single column vector $y^M$ with the model results at different time steps $i$:

$$y^M(\theta) = \begin{bmatrix} y^M_{i_1}(\theta), y^M_{i_2}(\theta), \ldots, y^M_{i_N}(\theta) \end{bmatrix}^T.$$  \(6\)

[29] Deviations between the simulation results of this deterministic model and measured data are due to measurement errors in output observations and due to errors in input, initial conditions, boundary conditions, and model structure that are propagated through the model. Because of this propagation of some of the errors through the model, we cannot assume the residual errors to be independent at different times even if the measurement process would lead to independent errors. In addition, we can expect all error contributions to be larger at large discharge than at small discharge. To consider this heteroscedasticity of the error term, we carried out a Box-Cox transformation [Box and Cox, 1964, 1982] as done by Schuwirth et al. [2008] and Yang et al. [2007] and rewrote the probabilistic output of the model as the vector of random variables:

$$Y^M = g^{-1}\left[\frac{y^M}{\lambda_0} + E_i\right].$$  \(7\)

where $E_i$ is the error term in transformed units and $g$ and $g^{-1}$ are forward and backward Box-Cox transformations given by

$$g(y) = \begin{cases} \frac{\left(y + \lambda_2\right)^{\lambda_1} - 1}{\lambda_1} & \text{for } \lambda_1 \neq 0, \\ \log \left(\frac{y + \lambda_2}{\lambda_0}\right) & \text{for } \lambda_1 = 0 \end{cases},$$

$$g^{-1}(z) = \begin{cases} \lambda_0 (\lambda_1 z + 1)^{1/\lambda_1} - \lambda_2 & \text{for } \lambda_1 \neq 0, \\ \lambda_0 \exp(z) - \lambda_2 & \text{for } \lambda_1 = 0. \end{cases}$$  \(8\)

[30] Here $Y^M$ is the vector of random variables representing the model result, $y^M$, including the stochastic errors. Parameters $\lambda_1$ and $\lambda_2$ are used to reduce heteroscedasticity and to make the error term $E_i$ approximately normally distributed, and $\lambda_0$ is used to make the expression in the parentheses dimensionless. It has a value of unity and the same units as the model result. To test the statistical assumption of the normal distribution of the error we analyzed the standardized residuals, $r$, of transformed data and model results

$$r = \frac{g(y^\text{obs}) - g[y^M(\theta)]}{\sigma}.$$  \(9\)

where $\sigma$ is the standard deviation of the error term $E_i$ in transformed units. The marginal prior probability density of $\sigma$ is assumed to be proportional to $1/\sigma$.

[31] To account for the autocorrelation of the residuals we applied a time continuous autoregressive error model [Yang et al., 2007]. It is assumed that the innovations, $I_i$, rather then the residuals, $E_i$, are independent,

$$I_i = E_i - E_{i-1} \exp\left(-\frac{t_i - t_{i-1}}{\tau}\right),$$  \(10\)

and normally distributed with a standard deviation of

$$\sigma_i = \sigma \sqrt{1 - \exp\left(-2 \frac{t_i - t_{i-1}}{\tau}\right)}.$$  \(11\)

where $t$ is the time and $\tau$ the characteristic correlation time.

[32] We expected the errors to be strongly autocorrelated in the recession part of the hydrograph, but only weakly during rain events. We therefore used two different correlation times for these two phases of simulation. During the recession phase, we set $\tau$ to 15 days and with each discharge that exceeded 1.5 mm d$^{-1}$ $\tau$ was reset to 1 day. To test the assumption of independency of the innovations we compared the standardized observed innovations of the transformed data and the transformed model results:

$$I_i = \frac{g(y^\text{obs}) - g[Y^M_i(\theta)]}{\sigma} - \frac{g(y^\text{obs}) - g[Y^M_i(\theta)]}{\sigma} \exp\left(-\frac{t_i - t_{i-1}}{\tau}\right),$$

$$\sigma_i = \sigma \sqrt{1 - \exp\left(-2 \frac{t_i - t_{i-1}}{\tau}\right)}.$$  \(12\)

where $\sigma$ is the asymptotic standard deviation of the error in transformed units that was also estimated during the calibration process.

[33] Combining the deterministic model with the Box-Cox transformation and the autoregressive error model leads to the following likelihood function [Yang et al., 2007]:
Table 2. Marginal Prior Distributions of the Percolation Rates and the Percolation Factors for the Modified Model Structure

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Parameter</th>
<th>Distribution</th>
<th>Mean</th>
<th>SD</th>
<th>Minimum</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Percolation Cambisol* (mm d⁻¹)</td>
<td>ρ₈₄ₑ₃₃</td>
<td>normal</td>
<td>0.5</td>
<td>2</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>Percolation Calcareous Cambisol* (mm d⁻¹)</td>
<td>ρ₈₄ₑ₃₃</td>
<td>normal</td>
<td>0.5</td>
<td>2</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>Percolation Dystric Cambisol* (mm d⁻¹)</td>
<td>ρ₈₄ₑ₃₃</td>
<td>normal</td>
<td>0.5</td>
<td>2</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>Percolation Cambisol-Pseudogley* (mm d⁻¹)</td>
<td>ρ₈₄ₑ₃₃</td>
<td>normal</td>
<td>0.25</td>
<td>2</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>Percolation Eutric-Gleysol* (mm d⁻¹)</td>
<td>ρ₈₄ₑ₃₃</td>
<td>normal</td>
<td>0.25</td>
<td>2</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>Percolation Gleysol* (mm d⁻¹)</td>
<td>ρ₈₄ₑ₃₃</td>
<td>normal</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>Percolation Wet Gleysol* (mm d⁻¹)</td>
<td>ρ₈₄ₑ₃₃</td>
<td>normal</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>Percolation Regosol* (mm d⁻¹)</td>
<td>ρ₈₄ₑ₃₃</td>
<td>normal</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>Percolation forest* (mm d⁻¹)</td>
<td>ρ₈₄ₑ₃₃</td>
<td>normal</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>Factor Cambisol* (1/d)</td>
<td>ρ₈₄ₑ₃₃</td>
<td>normal</td>
<td>0.45</td>
<td>1.8</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>Factor Calcareous Cambisol* (1/d)</td>
<td>ρ₈₄ₑ₃₃</td>
<td>normal</td>
<td>0.45</td>
<td>1.8</td>
<td>0</td>
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<td>normal</td>
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<td>normal</td>
<td>0.225</td>
<td>1.8</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>Factor Gleysol* (1/d)</td>
<td>ρ₈₄ₑ₃₃</td>
<td>normal</td>
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<td>1.8</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>Factor Wet Gleysol* (1/d)</td>
<td>ρ₈₄ₑ₃₃</td>
<td>normal</td>
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</tr>
<tr>
<td>Factor Regosol* (1/d)</td>
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<td>normal</td>
<td>0</td>
<td>1.8</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>Factor forest* (1/d)</td>
<td>ρ₈₄ₑ₃₃</td>
<td>normal</td>
<td>0.45</td>
<td>1.8</td>
<td>0</td>
<td>10</td>
</tr>
</tbody>
</table>

*The normal distributions are truncated at minimum and maximum; mean and SD refer to the means and standard deviations of the nontruncated distributions.

2.7. MCMC Sampling of Posterior Distribution

A sample from the posterior distribution (equation (5)) was derived by applying the Metropolis-Hastings Markov chain Monte Carlo (MCMC) algorithm [Gelman et al., 2004] using UNCSIM [Reichert, 2005, 2006]. We included in the analysis 47 parameters for the original model and 51 for the improved model (see section 2.4 and Tables 1–3). To avoid a burn-in phase, first a parameter optimization to maximize the likelihood was carried out. We used the algorithm SCE-UA [Duan et al., 1993] implemented in UNCSIM. The Markov chains were started at the best estimate of the position of the maximum of the posterior obtained from the optimization algorithm. The normal jump distribution was updated iteratively as recommended by Gelman et al. [2004]: On the basis of preliminary runs, the covariance matrix of the jump distribution was taken to be proportional to the preliminary estimate of the posterior and the scale of the distribution was adjusted to get a rejection rate of about 0.8. For the final runs, the jump distribution was no longer adjusted to guarantee convergence. Several chains were executed in parallel to compare their convergence. Convergence was tested by graphical analysis of the Markov chains, by a comparison of marginal densities of the chains, and by checking the posterior pdf values (of being close to the maximum). Our approach of not adapting the jump distribution during the final runs is still recommended by Gelman et al. [2004] to avoid possible convergence problems [Roberts and Rosenthal, 2007; Andrieu and Thoms, 2008]. However, adaptive MCMC algorithms that are carefully designed to converge may outperform this approach [Haario et al., 2001, 2006; Andrieu and Thoms, 2008; Vrugt et al., 2008, 2009].

2.8. Testing Spatial Predictions

The field study described by Leu et al. [2004a, 2004b] provided relative herbicide loss rates $L_{rel}$ (percentage of herbicides lost, $M_{loss}$ per mass applied, $M_{app}$) at the level of three subcatchments $j$:

$$L_{rel} = \frac{M_{loss}}{M_{app}} \times 100\%$$

Very pronounced spatial differences regarding $L_{rel}$ were observed (0.14%, 0.4%, and 0.02%; 56-fold difference between the extremes). Despite these differences, no difference in the timing of herbicide peak concentrations could be observed [see Gomides Freitas et al., 2008, Figure 6] irrespective of the compounds investigated (no measurable retardation). These results strongly suggested that the loss rate was mainly controlled by the convective transport of fast runoff generated on the corn fields that reached the stream either directly or via macropores and tile drains [Leu et al., 2004a, 2004b]. Since the flux into macropores and tile drains strongly depends on how much water flows laterally toward the macropores [Weiler and Naef, 2003; Stamm et al., 2002; Flühler et al., 1996] we assumed
that the herbicide loss was proportional to the volume of fast flow generated on the corn fields within the respective subcatchment that actually reached the stream. In the model, relevant fast flow from the corn fields was surface runoff directly connected to the stream, \( Q_{\text{surf,con}} \), and surface runoff that was intercepted by macropores on drained sink areas, \( Q_{\text{surf,sink}} \).

\[
L_{\text{rel}} \propto (Q_{\text{surf,con}} + \psi Q_{\text{surf,sink}}), \quad (15)
\]

where \( \psi \) is a proportionality factor, which accounts for the potentially different herbicide concentrations in directly connected surface runoff and the transport via tile drains. \( \psi \) is assumed to be constant across the catchment.

[37] Therefore, the spatial prediction does not require a specific herbicide transport model; it suffices to rely on a hydrological model as used here. For the actual comparison, we focused on the main herbicide loss event during the field study 2000.

3. Results and Discussion

3.1. Uncertainties in Discharge Prediction

[38] When propagating prior parameter uncertainty, we can hardly have information about the joint effect of model structure, input and observation error described by the autoregressive error model. For this reason, we show only prediction uncertainty bands due to parameter uncertainty in Figure 4a. Even when keeping in mind that the uncertainty ranges in this figure do not include model structure, input and observation error it becomes evident that the simulation shows significant systematic deviations from the observations. In particular, the base flow is strongly overpredicted and the peaks are underpredicted by the model. In addition, there is the striking observation that the prior prediction based on best estimates of the model parameters is often not covered by the 90% uncertainty interval. This is caused by the use of truncated distributions, especially for the percolation rates into the base flow reservoir. For the prior prediction, some percolation rates, for example for Gleysols and Regosols, were set to zero. The corresponding prior marginal is a normal distribution with mean zero truncated at zero. This truncation shifts the mean from zero to a positive value and causes a poorer fit.

[39] In contrast to the prior simulation, the 90% uncertainty interval of the calibrated original model (Figure 4b) is larger and brackets the measurements during the whole investigation period. The larger uncertainty is caused by the error model, which besides parameter uncertainty also accounts for errors in measurements, input data and model structure. Furthermore, the maximum and median of the posterior density are in good agreement. Both have Nash-Sutcliffe coefficients of 0.90, which is slightly higher than in the prior simulation. However, the base flow remains overestimated.

3.2. Restriction of the Parameter Distribution

[40] For the general model parameters \( \kappa \) and \( M_{\text{sink}} \) and for some of the percolation rates the widths of the posterior marginals became considerably smaller upon calibration with the discharge data (Figure 5). For example, little prior information was available for \( M_{\text{sink}} \) and the calibration largely reduced the uncertainty range. Similarly, the relatively high prior uncertainties of the percolation rates, per., of Gleysol, wet Gleysol, and Cambisol were substantially reduced. The posterior confirmed the prior expectation that Cambisols, which are pedologically characterized as well drained, have larger percolation rates than poorly drained Gleysols. The macropore parameter \( \kappa \) tended to be somewhat higher than in the reference study of Boll et al. [1998], but overall, it remained in the same range. In contrast, the prior and the posterior marginal probability densities of the hydrological soil parameters were very similar (Figure 6). This demonstrates that hardly any information was gained for them during the calibration procedure.

3.3. Residual Analysis of the Prediction of the Calibrated Original Model

[41] The residuals and innovations of the maximum posterior model result were analyzed to test the statistical assumptions (normally distributed and independent innovations) underlying the likelihood function (Figure 7).

[42] Comparing the normalized residuals of the original model before and after Box-Cox transformation (Figure 7a) demonstrated a reduced heteroscedasticity and a more homogenous distribution of the variance after Box-Cox transformation using transformation constants \( \lambda_1 = 0.3 \) and \( \lambda_2 = 0.05 \text{ mm d}^{-1} \). The normalized residuals are strongly autocorrelated, i.e., negative residual values are mostly followed by another negative value and positive values by another positive value (Figure 7c). The sequence of innovations of the error model (below) shows much more random variation and demonstrates the usefulness of the error model. However, during two dry periods (beginning and middle of the calibration period), the innovations still show strong autocorrelation. Furthermore, the normalized residuals at low measured discharge are predominantly negative. These observations correspond to the overpredicted discharge during low-flow periods using the original model.

[43] These systematic patterns in the time series of the innovations strongly point to model structure deficiencies. Overall, the simulated discharge amplitude was too small: the flow rate is overpredicted during low flow and underpredicted during peak flow. The model underestimates the catchment response to soil moisture conditions and shows a too linear reaction to input.

3.4. Improvements of the Model Structure

[44] One factor causing this weak response to rainfall is the assumption of constant hydraulic gradients, which are equal to the surface slope (except for drained areas). This corresponds to the kinematic wave approximation, which we considered to be a reasonable starting point for modeling the shallow hillslopes as found in the study area. However, nonlinear and dynamic gradients may exert strong effects on the discharge response in the (flat) drained fields and in proximity to the stream. Since these effects contribute to the subgrid variability for computationally realistic spatial discretization (i.e., 25 m by 25 m) we incorporated them into the improved model by replacing the constant percolation rate by a dynamic percolation rate (\( \text{per}_{\text{dynam}} \)) that changes with the height of the water table, \( h \), by introducing a soil-specific factor, \( f_{\text{soil}} \) (see section 2.3). Similarly,
Figure 4. Comparison of the measured and the simulated discharge, including 90% prediction uncertainty band, for the study catchment during the spring period in 2000. (a) Prediction based on prior information, (b) posterior prediction by the original model calibrated using discharge data, and (c) posterior prediction by the model with improved structure calibrated using discharge data. Median and quantiles were calculated at every time step, and the maximum posterior probability density was determined for the whole calibration period.
the hydraulic gradient on drained soil was made dependent on the water table.

[45] These changes in model structure yielded the expected results: base flow and peak discharge could be better simulated (Figure 4c). These improvements can be seen best upon inspection of the innovations and residuals (Figures 7b and 7d). Both time series are less autocorre- lated and show mainly a random distribution.

[46] The structural improvement of the model had dra- matic effects on the parameter estimates. In contrast to the original model, the marginals of general, percolation-related (Figure 5) and soil type specific parameters (Figure 6) were heavily constrained. Furthermore, $M_{\text{sink}}$ was estimated clearly higher than in the original model, the macropore parameter $\beta$ somewhat lower. The percolation factors strongly depended on soil type: soils that are pedologically considered to be well drained had maximum posterior percolation factors that ranged between 0.36 and 1.6 d$^{-1}$, while those of soils classified as poorly drained ranged between $4 \times 10^{-2}$ to 0.23 d$^{-1}$. The standard deviation of the error $\sigma$ represents the aggregated error of the simulation and is of high interest. Its marginal posterior was nearly halved using the improved model as compared to the original model. This indicates a significant reduction in model structural error achieved by the revised model structure.

[47] The narrow bands of the posterior marginals indi- cate a good identifiability of the parameters with the improved model structure. Nevertheless, the calibration caused part of the parameters to be strongly correlated, either negatively or positively. Most of the high correlations are related to parameters of the soil type Cambisol, which is most widespread in the catchment. This suggests a (par- tial) identifiability problem of parameters within a confined range of parameter values.

3.5. Uncertainties of Spatial Predictions

[48] To investigate the uncertainty of the spatial prediction and compare it with measured herbicide loss patterns, the discharge event of 31 May 2000 was chosen, because it
was the first major discharge event after herbicide application causing the largest herbicide losses [Leu et al., 2004a].

The prior prediction indicated a very high uncertainty in spatial prediction (Figure 8a). At the 5% quantile, as well as at the median, only very few, mainly sealed areas, which are not relevant for herbicide losses, were predicted to contribute to surface runoff. In contrast, at the 95% quantile most parts of the catchment produced surface runoff and were therefore prone to herbicide losses. Hence, while the parameter uncertainty caused only a rather small
uncertainty range for the discharge prediction (see Figure 4a), it caused extremely wide uncertainty bands for the spatial predictions.

This large uncertainty was slightly reduced by calibrating the original model (Figure 8b). There are areas that contributed to surface runoff in all simulations and others that never contributed to surface runoff within the 95% confidence interval. The spatial patterns were influenced by land use (no runoff in forests), the presence of subsurface drainage systems and topography.

The improvements in model structure had a large effect on the spatial uncertainty (Figure 8c). The area of surface runoff was larger at the 5% quantile and much smaller at the 95% quantile compared to the original version. Overall, the surface runoff prediction of the improved model agreed closely with the spatial distribution of the poorly drained soils (compare Figure 2b).

### 3.6. Comparison With Measured Herbicide Loss Patterns

The spatially distributed model response was evaluated by predicting fast flow from fields grown with corn during a field study and comparing it to the measured herbicide loss rates from these areas (see section 2.8). According to equation (15) the ratios of herbicide loss between subcatchments should correspond to the ratios of fast runoff generation if the connectivity to the stream network is accounted for.

This comparison yielded mixed results. All models (prior, calibrated original and improved model) predict highest amounts of surface runoff for subcatchment 2 and very little fast flow for subcatchment 3, in agreement with the observed losses (Figure 9). This agreement between the models, despite different spatial predictions (see above), stems from the fact that (1) the connectivity was the same for all of them and (2) all of them predicted little runoff generation in subcatchment 3 because of a very sandy subsoil [Frey et al., 2009].

The models differ in the predictions for subcatchment 1. While the prior prediction showed a good agreement with the observations, the calibrated models either significantly overpredicted or underpredicted the losses from this part of the catchment. The calibrated original model did hardly simulate any fast flow, while the improved

![Figure 7](image-url)
The model predicted the highest amounts for this area. The deviations seem to suggest that model modification did not improve the spatial prediction. However, because there was no direct connection on the surface in subcatchment 1, it is evident that all flow paths of the fast flow reaching the stream consist of macropore flow to subsurface drains. Hence, the model needs not only to make a correct prediction regarding runoff formation (causing possible ponding in the sink areas), but it has also to describe correctly how much of the surface runoff reaches the stream from the sinks as event water.

On the basis of the lack of any observed herbicide retardation [see Leu et al., 2004a] we set the herbicide flux equal to the macropore flow $\psi = 1$ in equation (15). Since $\psi$ cannot be estimated only on the basis of discharge data the comparison between simulations and observations critically depends on how reasonable the (spatially invariant) assumption of $\psi$ equals one actually is. On the basis of field studies, Kladivko et al. [2001] stated that herbicide concentrations in subsurface drains are often lower than in surface runoff. Hence, one could conclude that the improved model was successful in predicting the volumes of runoff formation in all three subcatchments but overestimated the proportion of herbicides that was quickly transmitted to the stream via preferential flow to tile drains (affecting mainly subcatchment 1).

Figure 8. The 5%, 50%, and 95% quantiles of the simulated spatially distributed surface runoff in the study catchment on 31 May 2000 for (a) the prior simulation, (b) the calibrated original model, and (c) the calibrated improved model.
3.7. Critical Evaluation of the Spatial Prediction

The spatial patterns of CSA predicted by the three models differed substantially (Figure 8) despite fairly similar discharge predictions (Figure 4). Similar observation were already made by Grayson et al. [1992] or specifically for the spatial prediction of CSAs by Easton et al. [2008]. In the following, we evaluated these results qualitatively on the basis of field observations on the occurrence of surface runoff.

The improved model predicted much more restricted critical areas than both others and the spatial distribution of soil types was clearly one of the controlling factors. The parameter uncertainty caused much less spatial variability of the CSA prediction: instead of different spatial extensions of the CSAs, as for the original model, the parameter uncertainty mainly affected the volume of runoff generated on the CSAs. Overall, the improved model predicted fast flow basically from poorly drained soils while the original model hardly yielded such a dependency on soil types. Hence, the improved model seems to make more sense in terms of hydrology. Furthermore, the calibrated original model predicted little runoff from subcatchment 1, which contradicts the observations of extended ponding in that area during major discharge events [see Frey et al., 2009, Figure 3]. The simulations of the improved model agreed much better in this regard.

The results presented so far demonstrate how sensitive the spatial predictions may depend on the underlying model structure used for the simulations. This outcome raises the question of what the model outcome would look like if additional model processes were included. SMDR and its improved version rely on certain simplifying assumptions and process representations as for evapotranspiration, macropore flow or lateral subsurface flow. The assumptions regarding lateral flow are most critical for the spatial CSA predictions. It is evident that the processes are more complex and dynamic than simulated by the kinematic wave approximation and the modification introduced in the improved model. This is especially true close to the lower boundary of hillslopes [e.g., Beven, 1981]. An improved model simulation would not only require a more comprehensive conceptual representation but also a higher temporal and spatial resolution than what was feasible in this study. For the future, this needs to be addressed because it would allow for capturing the short-term hydrological responses in a better way.

In the context of this study, it is obvious to ask how the CSA would have looked like if the temporal resolution had been subdaily. We may give a tentative answer, if we consider the improved model as a reasonable representation. Since it predicts stormflow basically to be generated on poorly drained soils only, one can expect that the extend of CSAs would not expand dramatically if analyzed at higher temporal resolution. A higher temporal resolution may also change the detection of CSA because of Hortonian overland flow. Hortonian overland flow can hardly be simulated if average daily rainfall intensity is considered. In the past, this was interpreted as a reasonable simplification for the humid climate as in the study area. However, a recent field study demonstrated that Hortonian overland flow may also be a crucial process under these conditions [Doppler et al., 2011].

3.8. Convergence of Markov Chains

After convergence, the sample of the Markov chain is representative of the underlying stationary distribution which equals the posterior. It is often difficult to diagnose whether a chain has actually reached convergence. There are several diagnostic tools to test for convergence, but all of them may fail to detect convergence failure [Cowles and
Carlin, 1996]. We had the additional problem that the number of simulations was restricted because of our computationally demanding simulation. With the original model structure, 65,000 simulation runs could be carried out; with the modified structure there were four chains with 55,000 to 90,000 runs.

[61] For the original model, the posterior distribution seemed to be adequately sampled by the Markov chain. The chain covered the range of each parameter repeatedly and no trend could be observed (data not shown). Furthermore, for all parameters the best value of the optimization run was covered in the range of the maximum of the marginal distribution (Figures 5 and 6).

[62] For the Markov chains of the improved model, it was more difficult to achieve convergence. Simulation runs not starting close to the estimate of the mode of the posterior gained by the optimization algorithm did not converge to the optimal solution of the SCE-UA algorithm. The chains were rather trapped in local maxima and could not be used for the analysis. It was crucial to start chains close to the best numerical approximation of the mode. However, the four chains starting at the parameter values of the mode of the posterior seemed to be reliable. The marginal distributions of all four individual chains covered the parameter values of the best approximation to the mode and only minor improvements of the mode where found by the chains. The convergence of these chains was confirmed by the fact that the individual chains yielded similar marginals (not shown). For the analysis all four chains were then used jointly. Convergence of the Markov chains is a critical point for inference. A chain that has not converged has not adequately sampled the entire distribution. This would lead to an underestimation of posterior uncertainty.

[63] One factor that may contribute to these convergence problems are thresholds in process formulations of hydrological models. They can lead to complicated shapes of the posterior with many local optima [Kavetski et al., 2006; Kavetski and Kuczera, 2007]. Models used in this paper contain various thresholds (e.g., for the onset of surface runoff) and it would be a good option to smooth these thresholds in the future. This also applies to thresholds that are physically based. For example, macro pore activation is generally described by a threshold function. However, because of the large heterogeneity of the soil and the spatial resolution of the model being much larger than the scale of the physical threshold processes (e.g., infiltration into a single macro pore) a smoothed threshold may be more realistic.

[64] It is a general problem that computationally demanding simulation models are restricted in their use for computer-intensive analysis techniques like MCMC simulation. However, more complex problems, such as the prediction of CSA, require a spatially resolved model that is necessarily complex. For this reason, efficient model implementation is crucial, which is unfortunately not the case for SMDR. By rewriting of parts of the code, the simulation time could be drastically reduced. However, the program still needs 5 min for one simulation run on a 2.33 GHz CPU. A complementary strategy to overcome this problem is to use emulators. An emulator interpolates the predictions of complex models in parameter space [O’Hagan, 2006]. Emulators for dynamic models are still under development [Bhattacharya, 2007; Liu and West, 2009; Reichert et al., 2011]. Parallel computing of multiple Markov chains simultaneously would be another option [e.g., Vrugt et al., 2006].

4. Learning From Local Data

[65] The starting point of this study was the uncertainty analysis of CSA predictions that are solely based on data generally available to land managers like soil maps, land use, or topography. In subsequent steps, we investigated how the incorporation of additional local information in the form of measured discharge data allowed for improved predictions and decreased uncertainties within this particular case study. The overall structure of this procedure consisted of the following steps.

[66] 1. The first step is prior uncertainty prediction. Although the comparison between the prior discharge prediction and the observation revealed a reasonable agreement on the basis of the traditional Nash-Sutcliffe criteria, the measured discharge values often laid outside the 90% bands of the prediction based on prior information and the original model structure (Figure 4). Hence, during this first learning step, the use of local data clearly indicated that parameter uncertainties were not the only relevant source of uncertainty. Hence, other error sources needed to be incorporated in an appropriate error model for the subsequent inference step.

[67] 2. The second step is Bayesian updating of the original model. To account for these different error sources we incorporated an autoregressive error model into the Bayesian inference approach. This error model accounts for the effect of input, model structure, and measurement errors on the model output (stream discharge). This error model improved the agreement of measured discharge with statistical model assumptions considerably. Nevertheless, it has two major disadvantages: First, it lumps the effect of input, model structure and output errors together instead of providing separate estimates of these error contributions. Second, this statistical error description can only be identified for model outputs for which measured data are available. These are general disadvantages of all methodologies that correct for deficiencies in model structure, input and output by autoregressive error models or other bias correction terms in model output only [Kennedy and O’Hagan, 2001; Bayarri et al., 2007]. In the present application, this leads to an underestimation of uncertainty ranges of the identified CSA, as the autoregressive error model could only be identified for stream discharge. Approaches for identifying the different error contributions separately are making model equations stochastic [Vrugt et al., 2005], performing a “total error analysis” [Kuczera et al., 2006], or using time-dependent model parameters to identify model deficiencies and introduce stochasticity without violating conservation laws [Reichert and Mieletiuer, 2009]. However, all of these approaches are computationally very demanding and not feasible within the framework of this project.

[68] Learning from the data by this Bayesian updating procedure had two major, contrasting effects: first, the parameter uncertainty was decreased as seen from the constrained marginals of influential parameters like the percolation rates. Second, the updating resulted in posterior uncertainty bands that were substantially wider than for the prior predictions.
This was not the effect of possible correlations between parameters (these correlations were rather weak, data not shown), but the effect of the autoregressive error term.

For residual analysis and model modification, a careful analysis of the residuals and innovations (Figure 7) revealed systematic errors in the base flow calculation during dry periods that could not be accounted for by a modified error model. These deviations pointed to structural model deficiencies like the kinematic wave approximation used in the original model when applied to the study catchment. To improve the model for this application, we modified the code as described in section 3.4. Hence, checking the inference assumptions regarding residual distribution and innovations was an important step to improve the quality of prediction.

In Bayesian updating of the improved model, the conceptual modifications of the original model had strong effects regarding model performance, model uncertainties and the spatial predictions. First, the residual analysis demonstrated that the conditions formulated in the likelihood function based on the improved model structure are fulfilled. This follows from the fact that the simulations of the base flow dynamics could be improved significantly. Second, the Bayesian updating resulted not only in a high learning effect for the general model parameters and the percolation factors, as for the original model, but also for the hydrological soil parameters. In the original model, the percolation rates controlled the vertical water flow. The soil properties had hardly any influence. In the improved model, the percolation also depended on the hydrological soil parameters because they control the level of the water table. This clearly shows that the information content of local data may be dependent on model structure. Third, the updating of the improved model decreased the discharge prediction uncertainty substantially. This was caused by constraining the parameters much more than in the original model. Furthermore, the model structure uncertainties could also be strongly reduced as seen from the comparison of the error terms $\sigma$ of the respective models (Figure 5). Finally, the updating of the improved model had a very pronounced effect on the spatial predictions and their uncertainty, which was strongly limited.

The last step is to test with independent data. As a final point, the spatial predictions of all three models (prior prediction, calibrated original model, and calibrated improved model) were compared to the observed herbicide loss patterns from the three subcatchments. The comparison showed a partial agreement with the observations but also deviations (see section 3.6). The comparison also points to the limitations when only discharge data are available for calibration. Even though the generation of fast flow is a dominant factor for herbicide transport, discharge data do not provide insight into how macropore flow generates outflow of pre-event (without herbicides) or event water carrying herbicides (see equation (15)). Therefore, the herbicide loss data do not provide a sufficient basis for testing the model predictions in quantitative terms.

5. Conclusions

Catchment models are claimed to be crucial tools for decision support regarding land management in agricultural catchments. Different spatially distributed models like SWAT or SMDR have been used for that purpose in the past [Easton et al., 2008; Frankenberger et al., 1999]. It is important to note that for agricultural land management the application of catchment models needs to cover large areas. This is in contrast to local pollution and water quality studies that often only need small- or intermediate-size catchments to be modeled. In these cases, often information is available from site-specific investigations that provide good data for setting up a model. In contrast, large-scale application of catchment models for optimizing agricultural production and mitigation of diffuse pollution are generally based on very sparse data. Areal coverage of data usually only exists for topography and land use. Data for parameterizing hydraulic properties of the catchments generally need to be derived from proxy data. Hence, this problem is closely related to the problem of predicting the hydrology of ungauged catchments [Sivapalan et al., 2003].

The underlying assumption of using models for tackling such land management issues is that it is faster and cheaper to replace local measurements and observations by model predictions on the basis of generally available data. In this paper, we have tested this assumption (1) by investigating the uncertainty of such prior predictions and (2) by investigating how predictions change and can be possibly improved by learning from local data in a sequence of learning steps. Although our prior predictions agreed very well with the observations, it seems that this agreement is at least partially a fortuitous outcome. A closer investigation revealed substantial model structure errors that could be overcome (partially) in the subsequent learning steps.

Overall, the results lead to two important conclusions with regard to the relevance of local data and the use of models in the context of mitigating diffuse pollution at the scale of small catchments:

1. Local data on relevant fluxes and state variables are crucially important. Not the least relevance is that they build the basis for plausibility checks of the model predictions [see, e.g., Holländer et al., 2009].

2. The value of local data is strongly dependent on a correct model structure for which they are used. Hence an iterative procedure of Bayesian updating, model testing, and possible model modification is suggested.

Despite all these reservations regarding the use of models without local observations they are indispensable tools because they yield a consistent representation of processes conditional on the hopefully explicit assumptions that can hardly be obtained in another way.

Overall, the results from this study suggest that spatial predictions of CSAs for diffuse pollution without local observations supporting them (at least in qualitative terms) are rather uncertain. This might call for new ways of interaction between research and practice in order to make models the useful tools as we like to claim them from a scientific point of view. Instead of delivering model predictions that shall yield useful results for practitioners in a single step, we bring the learning steps described in this study to a larger level by forming a loop of mutual learning iterating between research and practice: Researchers provide prior predictions representing hypotheses maps regarding the location of CSAs. Local practitioners and authorities provide targeted (qualitative) local observations that can be...
used for Bayesian updating. Subsequent analysis of residuals and possible model improvement. Although this will be a formidable task to set up such a loop in practice, it may be a promising endeavor that could also profit from new sensor technologies that make spatial data much easier to obtain.

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