Prediction of critical source areas for diffuse herbicide losses to surface waters

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Contents

Summary vii

Zusammenfassung ix

1 Introduction 1

2 Predicting critical source areas for diffuse herbicide losses to surface waters: role of connectivity and boundary conditions 17

2.1 Introduction ......................................................... 18

2.2 Methods ............................................................. 21

2.2.1 Study area ...................................................... 21

2.2.2 Herbicide and discharge data ................................ 22

2.2.3 Model Description ............................................. 23

2.2.4 Input data ........................................................ 28

2.2.5 Quality criterion ............................................... 31

2.2.6 Sensitivity analysis ........................................... 32

2.3 Results ............................................................... 34

2.3.1 Surface Connectivity ........................................... 34

2.3.2 Discharge Prediction ......................................... 34

2.3.3 Soil saturation .................................................. 36

2.3.4 Spatial Prediction .............................................. 38

2.3.5 Sensitivity Analysis .......................................... 39

2.4 Discussion ........................................................... 42
2.4.1 Relevance of surface connectivity .......................... 42
2.4.2 A priori predictions: potentials and limitations .......... 44
2.5 Conclusion ....................................................... 45

3 Reduction of structural uncertainties in hydrological modeling using discharge data in a Bayesian Inference approach 53
3.1 Introduction ..................................................... 54
3.2 Methods ......................................................... 57
  3.2.1 Study area and calibration data .......................... 57
  3.2.2 Model ....................................................... 57
  3.2.3 Improvements of the model structure .................... 60
  3.2.4 Prior Parameter Estimates .................................. 60
  3.2.5 Uncertainty analysis of prior prediction ................. 61
  3.2.6 Bayesian Inference ......................................... 62
3.3 Results .......................................................... 66
  3.3.1 Uncertainties in discharge prediction ..................... 66
  3.3.2 Residual analysis of the predictions of the calibrated models ... 68
  3.3.3 Restriction of the parameter space ....................... 69
  3.3.4 Uncertainties of spatial predictions ....................... 72
3.4 Discussion ...................................................... 75
  3.4.1 Uncertainty of discharge prediction ...................... 75
  3.4.2 Potential of discharge to constrain the parameter space ...... 75
  3.4.3 Spatial prediction of critical source areas ............... 76
  3.4.4 Convergence of Markov Chain ............................ 77
  3.4.5 Conclusions ............................................... 78

4 Comparison of different models to predict hydrologically sensitive areas for herbicide losses 85
4.1 Introduction .................................................... 86
4.2 Methods ......................................................... 88
Summary

Field studies have shown that diffuse herbicide losses from agricultural fields to surface waters often originate from only a limited part of a given catchment. These critical source areas (CSA) are characterized by the occurrence of fast flow processes like surface runoff or macropore flow to tile drains. A reliable identification of CSA offers promising options for mitigation measures to reduce diffuse herbicide pollution of surface waters.

We tested the predictability of locating CSA with the physically based hydrological water balance model SMDR (Soil Moisture Distribution & Routing). The study area was a small agricultural catchment in Switzerland in which herbicide transport to surface waters had been investigated in field studies and a large spatial variability of herbicide losses was detected. SMDR was adapted to the local conditions by implementing a model for artificial drains and considering the connectivity to the stream.

The analysis of the connectivity revealed that surface runoff from a large part (66%) of the study area cannot directly reach the stream network. Small scale topographic barriers often interrupt the overland flow. The surface connectivity could be assessed using terrain analysis based on a high-resolution (2 m) digital elevation model (DEM). A high resolution DEM is mandatory for this analysis. Using a DEM with a resolution of 25 m leads to a large overestimation of the surface connected area because important topographic features like functional barriers are overlooked. Surface runoff from unconnected areas infiltrates in local sink areas. If the sink area is drained, surface runoff can still reach the stream via preferential flow paths (macropores in vertical and drains in lateral directions).

For a practical application, prior model parameters were assessed based on generally available data. The resulting simulated discharge agreed well with the measured values. The spatial distribution of CSA and predicted runoff processes can explain the spatial variability of the measured herbicide losses. The main losses are predicted for surface connected areas prone to overland flow; additionally, drained sinks are also
Topography was the main determinant for the spatial distribution of CSA, and not soil properties. Topography predicts CSA mainly along the stream. Furthermore, the prediction of CSA locations is sensitive to parameters describing the lower boundary of the soil, the spatial extent and the efficiency of the drainage system.

However, our predictions of CSA locations involve large uncertainties since the knowledge of the model parameters is coarse due to limited data availability. Besides parameter uncertainties, model structure uncertainty also plays an important role. We investigated to what extent river discharge data can improve the prediction of CSA locations by constraining parameter values.

Bayesian inference was applied to combine the prior knowledge used in the first study with river discharge data. To consider the effect of model structure and input uncertainty on calculated river discharge, we formulated the likelihood function with an autoregressive error model additive to the river discharge calculated by the deterministic hydrological model. Despite using such an error model, the residual analysis indicated remaining model structure deficits.

With additional improvements of the model structure we were able to reduce the model structure bias to a significant extent. Furthermore, in combination with the discharge data, the uncertainty in the prediction of CSA locations was substantially reduced.

In a final step, we compared the CSA locations predicted by six different approaches. Despite their conceptual differences, the spatial agreement in the prediction of risk areas was surprisingly high. Approaches relying on soil data or topography led to similar results indicating that topography is reflected in the soil distribution in this landscape. Overall, topography is the most important source of information for practical applications, since it allows for assessment of the connectivity and saturated areas prone to fast flow processes and is relatively easy to detect at a larger scale.
Zusammenfassung


Wir haben untersucht, inwiefern solche Risikogebiete mit einem physikalisch basierten hydrologischen Wasserbilanzmodell (Soil Moisture Distribution & Routing) vorhergesagt werden können. Unser Untersuchungsgebiet war ein kleines landwirtschaftliches Einzugsgebiet in der Schweiz, in dem der Herbizidtransport in das Oberflächengewässer vorgängig in Feldstudien untersucht worden war. Dabei zeigten diese Untersuchungen eine große räumliche Variabilität der Herbizidabschwemmung. Um die lokalen Begebenheiten zu berücksichtigen, haben wir das hydrologische Modell erweitert und zusätzlich den Abfluss durch das Drainagesystem und die Konnektivität zum Oberflächengewässer explizit berücksichtigt.

Untersuchungen zur Konnektivität haben gezeigt, dass der Oberflächenabfluss von einem großen Teil des Einzugsgebietes (66%) nicht direkt in das Gewässersystem gelangen kann, weil kleinräumige topographische Barrieren den Abfluss verhindern. Die Konnektivität innerhalb des Einzugsgebietes konnte mittels Geoinformationssystemanalysen der Oberfläche basierend auf einem hoch aufgelösten Geländemodell (2 m) abgeschätzt werden. Analysen basierend auf einem Geländemodell mit einer Auflösung von nur 25 m führten zu einer großen Überschätzung des oberflächlich verbundenen Gebietes, weil entscheidende topographische Hindernisse darin nicht abgebildet waren. Oberflächenabfluss aus nicht verbundenen Gebieten fiesst in lokale Senken, wo das Wasser in den Boden infiltriert. Wenn die Senke künstlich drainiert ist, kann der Oberflächenabfluss das Oberflächengewässer über präferentielle Fließwege immer noch vergleichsweise schnell erreichen. In vertikaler Richtung führen Makro-
poren zu präferenziem Fluss, für den lateralen Transport ist das Drainagesystem verantwortlich.


Die räumliche Ausdehnung der Risikogebiete wurde hauptsächlich durch die Topographie bestimmt; Bodeneigenschaften waren weniger wichtig. Risikogebiete befanden sich größtenteils entlang des Baches. Die Modellierung von Risikogebieten ist sensitiv auf Modellparameter, welche den unteren Rand des Bodenhorizontes beschreiben und auf Parameter, die die räumliche Ausdehnung sowie die Effizienz des Drainagesystems bestimmen.


Durch zusätzliche Verbesserungen in der Modellstruktur konnten wir den Modellstrukturfehler signifikant reduzieren. In Kombination mit einer Kalibrierung basierend auf den Abflussdaten konnte auch die räumliche Unsicherheit in der Risikogebietsvorhersage substanziell reduziert werden.

In einem letzten Schritt haben wir die räumlichen Vorhersagen von Risikogebieten von 6 verschiedenen Modellen verglichen. Trotz ihrer konzeptionellen Unterschiede zeigten diese Modelle eine überraschend grosse Übereinstimmung in der räumlichen Vorher-
Chapter 1

Introduction
In modern agriculture, the use of herbicides is a common practice to increase productivity. According to the U.S. Environmental Protection Agency, pesticides are substances intended to prevent, destroy, repel, or mitigate any pest (U.S. EPA, 2009). Herbicides are compounds that are designed to eliminate weeds, but may also affect non-target species depending on their selectivity (Ecobichon, 2001). As long as herbicides remain in the top soil of a treated field, they behave as intended and have no impact on the aquatic environment. However, through different processes, herbicides may be transported off of the application site and spread further into the environment where they may impair the ecosystem. Herbicide contamination has been reported in groundwater (e.g. Loague et al., 1996), surface water (e.g. Wauchope, 1978), sediment (e.g. Devault et al., 2007) and the air (e.g. Richards et al., 1987).

Various laboratory and field studies have reported the impact of herbicides on non-target organisms. For example, Battaglin and Fairchild (2002) evaluated the potential toxicity of herbicide mixtures measured in streams from agricultural areas during runoff events. Thereby, some samples showed a probable toxicity to plants and algae. Giddings et al. (2000) also concluded a certain risk for invertebrates. Effects on higher organisms like frogs or fish are less likely (Solomon et al., 2008). However, this conclusion is discussed controversially, compare correspondence of Solomon (2009), Collins (2009) and Hayes (2009). Furthermore, a negative correlation between aquatic species diversity and the risk of herbicide pollution have been reported (e.g. Probst et al., 2005; Liess and Von der Ohe, 2005). Drinking water can also be affected by herbicides as discussed in Tesfamichael et al. (2005).

Herbicide contamination is also an issue in Switzerland. Since the reform of Swiss agriculture in 1992, the policy has been focused on a market-based and ecologically oriented agriculture. The income of the farmers has been decoupled from the product price and the farmers are subsidized by direct federal payments, as long as they fulfill a minimum set of agro-ecological requirements. Concerning herbicides, the overall political goal was to halve the pesticide loads in surface waters by 2005 compared to the reference years 1990 to 1992 (BLW, 2001; Flury, 2005). This should be achieved by a 30% reduction of the applied amounts (implementation goal) along with improved management measures that minimize the transport of the applied herbicides into the environment (effect goal). Due to the uncertain data base and the temporal delay of the reduction towards the implemented measures, only a limited and simplified evaluation of these goals was possible. Singer et al. (2005) concluded that a reduction of the applied herbicides amount was achieved. However, it is unclear to what extent new highly potent herbicides are responsible for this trend because they require considerably lower application rates. In contrast, the effect goal could not be achieved. Singer et al.
(2005) could not detect a herbicide reduction in the environment that goes beyond the effect caused by deceased application amounts.

Two different agricultural sources of herbicide pollution are observed. On the one hand, herbicide losses originate from point sources like farmyards (e.g. Kreuger, 1998; Carter, 2000) where herbicides were handled improperly during cleaning or filling of sprayers. In some regions, point-sources are responsible for the majority of the observed pesticide loads (e.g. Muller et al., 2002). Even if point sources do not account for a major part of the total load, they may still lead locally to high peak concentrations that are of toxic relevance (Leu et al., 2004a). To reduce these losses, the herbicide users must become more aware of this problem and improve the proper handling and application of herbicides (e.g. filling and cleaning of the sprayers only on fields or biobeds and replacing defective or outdated spray equipment, cf. Reichenberger et al., 2007).

On the other hand, herbicide pollution may also originate from diffuse sources from agricultural fields. Diffuse pollution is usually defined as inputs into water bodies resulting from agricultural applications (e.g. Reichenberger et al., 2007). Paths for herbicides into surface waters include: overland flow; tile drains; subsurface flow; soil erosion; spray drift during applications; and deposition after volatilization. In contrast to point sources, diffuse losses are more difficult to deal with since the pollution can not be directly traced back to a well defined origin. Therefore, it is still a challenge to implement effective measures to reduce or prevent pollution from diffuse sources (Campbell et al., 2004).

The terms diffuse and non-point source are somewhat misleading. Several studies have shown that not all parts of a catchment contribute to diffuse pollution to the same extent and the majority of herbicide pollution originates from distinct and limited areas (Blanchard and Lerch, 2000; Leu et al., 2004b; Gomides Freitas et al., 2008). This identified spatial variability of the risk areas for herbicide pollution is the motivation of this work. Mitigation options that focus on those risk areas have a large potential to effectively reduce herbicide pollution to surface waters. Options like well placed buffer strips or avoiding herbicide application on high risk areas would lead to a further reduction of herbicide contamination as it is intended by the Swiss agricultural policy without constraining the economical scope of the farmers. Therefore, the main question of this work is: how can we identify such risk areas in advance and what catchment attributes can be used to identify them?

Herbicide transport processes from agricultural fields are tightly linked to the hydrology of those fields. Hydrological transport processes are primarily responsible for the mobilization of the applied herbicides in the soil and their distribution and transport to
surface waters. It has been demonstrated that herbicide transport occurs primarily during and shortly after rain storm events that lead to an increased discharge (Leu et al., 2004a). Thereby, fast flow processes are mainly responsible for the transport of herbicides to water bodies. The transport through the soil matrix is less important because degradation and sorption take place during that slow transport. The highest amount of herbicide losses occur during rain events shortly after the application when less of the applied herbicides have been sorbed or are degraded (e.g. Crawford, 2001; Gomides Freitas et al., 2008).

The two dominant fast flow paths for herbicide losses are surface runoff and preferential flow through macropores and the drainage system (e.g. Flury, 1996; Carter, 2000). Two different surface runoff processes are distinguished: infiltration excess, also called Hortonian overland flow; and saturated overland flow. Hortonian overland flow occurs when the precipitation intensity exceeds the infiltration capacity of the soil (Horton, 1933). Saturated overland flow occurs when the water table rises to the surface and generates overland flow (Dunne et Black, 1970). In the humid and well-vegetated Swiss midland areas, saturated surface runoff is the dominant process. Hortonian flow occurs only during very intensive rain storm events or on areas with reduced infiltration capacity (e.g. due to soil compaction or surface sealing).

Fast transport through macropores and artificial drainage systems can also be important. Stamm et al. (2002) concluded that the distinction between surface runoff and drainage flow is not well defined. Water often moves laterally as surface or near surface runoff before it is intercepted by macropores, channeled into the soil and transported through the drainage system to surface water. Overall, we can conclude that fast flow processes are mainly generated on saturated areas.

A further possible transport process, primarily for pesticides that are strongly adsorbed, is erosion (e.g. Wauchope, 1978). Erosion can be distinguished as two separate processes, the detachment of soil particles from the soil surface and the subsequent transport to surface water. The detachment is triggered by raindrops or by surface runoff. Surface runoff is then responsible for the transport of the particles to surface water (Morgan, 2001). Hence erosion is strongly connected to surface runoff. Therefore, areas vulnerable to erosion are in general also risk areas for surface runoff.

In hydrology, the idea that only a limited part of a catchment produces fast flow during storm events has been known for decades (partial area concept Betson, 1964). Furthermore, Hewlett and Hibbert (1967) described the shrinking and expanding of those areas in their variable source area concept. Similar ideas were simultaneously developed by Cappus (1960) in France and by Tsukamoto (1963) in Japan. The concept is
also relevant for diffuse pollution since the source areas also initiate herbicide transport. For example, Qiu (2003) proposed to install conservation buffers based on the hydrology of variable source areas.

Ambroise (2004) extended the variable source area concept by introducing “active” and “contributing” areas. Active areas are all areas producing fast flow equivalent to variable source areas. However, not all active areas necessarily contribute to the output at the catchment outlet. Whether an active area is contributing depends on the hydraulic connections between active areas and the catchment outlet.

Two useful approaches to identify risk areas for diffuse pollution based on the variable source area concept are the hydrologically sensitive areas (HSA) and the critical source areas (CSA). HSA are all areas in a watershed that are prone to generate runoff and therefore potentially susceptible to contaminant release (Walter et al., 2000). CSA are HSA that additionally contain pollutants that are available for transport (Pionke et al., 1996). In our work we mainly use the term CSA in the chapters 2 and 3 and the term HSA in the chapter 4. In the past, these approaches were often applied for management of phosphorus losses (e.g. Gburek and Sharpley, 1998; Gburek et al., 2000; Pionke et al., 2000; Heathwaite et al., 2005; Gerard-Marchant et al., 2006; Lazzarotto et al., 2006). Since phosphorus has similar fast transport pathways in soils as herbicides, these approaches are also interesting for the study of herbicide pollution.

The variable source area concept is not without controversy. McDonnell (2003) challenged the underlying assumption of model structures based on the variable source area concept. His concerns about the topographically defined flow paths, the linear wetting in hillslopes, the uniform relation between groundwater storage and runoff for the whole catchment, and the assumption that all relevant processes take place in the soil mantle must be considered in variable source modeling. Despite these critical points, the variable source area concept still captures the major aspects of runoff formation. Fast flow contributing areas are spatially limited and their extent is variable in time.

Compared to the hydrological characteristics of the fields, substance properties like sorption behavior of mobile pesticides are less important for the spatial variability of the herbicide losses (Stamm et al., 2004). Leu et al. (2004a) showed that the relative losses of three investigated herbicides atrazine, dimethenamid, and metolachlor did not vary by more than a factor of three in contrast to a spatial variability of over fifty caused by catchment intrinsic parameters. Gomides Freitas et al. (2008) confirmed these findings additionally for sulcotrione, which is an acidic herbicide in contrast to the neutral compounds studied by Leu et al. (2004a). Thus, a CSA for one herbicide
is generally a CSA for another herbicide, as long as they are applied to similar crops. Therefore, a prediction of CSA can focus on the spatial variability of hydrological fast flow processes.

For that purpose, a spatially distributed modeling approach is needed. Spatially distributed modeling has been an important issue in hydrology for many years, but despite increasing computer power, modeling hydrological processes within catchments still remains a challenge. This holds especially true for fast flow transport processes, since a large number of factors interfere.

Already in the 1960s, Freeze and Harlan (1969) published a blueprint for a comprehensive spatially distributed hydrological model. They predicted that, based on physical principles, a universal applicable hydrological model should soon become available. However, nowadays such universal hydrological models are still not available. Beven (2002) pointed out that, unlike other fluid dynamic disciplines (e.g. meteorology, oceanography), hydrology is dominated by conditions on quite a small-scale and flow processes are largely dominated by the local geometry, local soil conditions, and boundaries rather than the dynamic of the fluid itself. Hydrological transport processes are well understood at the very small scale (size of about 0.1 m), however the scale of a typical herbicide application is usually much larger. A model structure valid at small scale is only expected to be valid on that limited scale. To apply it at a larger scale such as on agricultural fields or small catchments will require an enormous amount of input data with a small scale resolution. However, based on the current state of measurement technology, this is not possible. Roth et al. (1999) stated that there is a need for an effective process model based on effective material properties that retain the essential features of the phenomenon of the small scale. There exist different competing effective process models. Beven (2002) stated that an adequate model should be based on physical principles (e.g. mass conservation) and should be consistent with observations. Therefore, we were seeking a hydrological model that incorporates all relevant processes for herbicide transport typically occurring in the type of landscape we are working in.

Our study site is a small agricultural catchment within the Swiss Plateau with a moderate topography. Previous investigations in the area confirmed that saturation-induced surface runoff and preferential flow are the dominant processes causing herbicide transport to surface waters (Leu et al., 2004a; Schmocker-Fackel et al., 2007). Furthermore, large parts of the catchment area are artificially drained. Based on our requirements and the catchment conditions, we chose the Soil Moisture Distribution and Routing (SMDR) model which is based on the variable source area concept (Boll et al., 1998;
Soil and Water Laboratory, 2003). SMDR is a fully distributed, physically based hydrological model with the objective of identifying the locations and the temporal variability of HSA. It accounts for surface runoff and macropore flow and in a previous application an artificial drainage system was included (Frankenberger et al., 1999). Furthermore, its open source code allows users to incorporate additional processes such as the consideration of surface connectivity.

Spatially distributed models are in general very parameter intensive, which is often in contrast to the actually available data. To limit the number of parameters, hydrological response units can be introduced (e.g. Flügel, 1995). Hydrological response units are areas that are parameterized in the same way, as a result of similar properties such as specific topographic and/or soil type characteristics. The underlying assumption is that hydrological differences within the same hydrological response unit are much smaller compared to other units.

A further difficulty of spatially distributed models is their validation against observed data, since current hydrological data collections are commonly limited to catchment outlets (Srinivasan and McDowell, 2007). Due to previous intensive field investigations (Leu et al., 2004a,b, 2005; Gomides Freitas et al., 2008), we have quantitative data on the spatial heterogeneity of herbicide losses for three subcatchments within the study catchment. The exact knowledge about the herbicide application data and spatially distributed measurements of herbicide concentrations during a controlled field study allowed us to test our model predictions.

For practical application, the prediction of CSA locations has to be based on available data; extensive field investigations to derive all model parameters are not possible. In chapter 2, we investigated the predictability of CSA locations for our catchment based on available data without calibration and a physically based hydrological model in a case study. In order to understand how spatial prediction may be improved in the future, we analyzed the factors which caused the spatial variability of herbicide pollution and studied the sensitivity of the model towards the model parameters.

The sensitivity analysis revealed that the prediction of CSA locations is sensitive to parameters for which only little information is available (e.g. lower boundary conditions of the soil profiles). The uncertainties in these parameters are propagated by the model and lead to large uncertainties in the spatial prediction.

However, model parameters are not the only source of uncertainties. There also is a high structural uncertainty about the model formulation. A mathematical model is necessarily a simplified representation of reality. There are uncertainties as to whether all relevant variables and processes are incorporated, uncertainties about the choice of
the spatial and temporal model resolution, and uncertainties about the underlying model assumptions of the model formulation. Furthermore, there are uncertainties about the driving external input factors (e.g. rainfall data), the observed validation data, or even in the numerical solution (Beck, 1991; Kennedy and O’Hagan, 2001).

For practical implementation of mitigation and management strategies, it is crucial to reduce the uncertainties as much as possible and to communicate them correctly to stakeholders. To reduce the uncertainty, additional calibration data are necessary. However, such calibration data are often limited for practical application. Discharge is the most typical calibration data available since it can be measured in a relative simple way. Discharge data integrates information from the entire catchment; therefore their spatial differentiation is limited. We investigated in chapter 3 to what degree discharge data can help to decrease the prediction uncertainty.

There are differing philosophies on uncertainty analyses within hydrological models (e.g. discussion of Mantovan and Todini, 2006; Beven et al., 2008). We applied a Bayesian inference approach which allowed us to incorporate different sources of uncertainty in the calibration process (Kennedy and O’Hagan, 2001; O’Hagan, 2003; Bayarri et al., 2007). Furthermore, spatially distributed models are in general very parameter intensive and their calibration often leads to parameter non-uniqueness. In the Bayesian context, non-uniqueness, also called equifinality, is not a limitation as it occurs automatically when the posterior is flat in certain directions. In a Bayesian approach, prior information is combined with observed calibration data. The updated posterior probability distribution of model parameters and results reveals to which degree the data reduced the uncertainty compared to the prior knowledge. The Bayesian approach also allows an accounting of different sources of uncertainty by combining the likelihood function with an adequate error model.

To test the statistical assumption of the inference processes, a residual analysis was carried out. The investigation revealed some systematic deviation between model results and observation. To reduce that systematic deviation and to improve the agreement between the residuals (and innovations) and the statistical assumptions, the model structure had to be improved. In chapter 3, we also described these adaptations and how they affect the calibration process and the prediction uncertainty.

The uncertainty analysis highlights the importance of the model structure. There are different competing model structures to predict HSA areas. In the chapter 4, we compared different approaches. Thereby, we focused our comparison on simple approaches that may be easily applied in practice. These approaches are useful for the application on a larger scale, since physically based models are, due to their complexity and time
consuming implementation, often not applicable on a larger scale. Besides SMDR, we considered the FAL risk map of the local soil map (FAL and Kanton Zürich, 1996), the Dominant Runoff Processes (Scherrer and Naef, 2003; Schmocker-Fackel et al., 2007), the HOST approach (Boorman et al., 1995), a regression model for the fast flow index (Siber et al., 2009), and the topographic (wetness) index (Beven and Kirkby, 1979).

In the last chapter 5 the thesis finishes with a short conclusion of the previous chapters and an outlook on future research topics.
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Chapter 2

Predicting critical source areas for diffuse herbicide losses to surface waters: role of connectivity and boundary conditions

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Abstract  Field studies have shown that diffuse herbicide losses to surface waters often originate from a limited part of a catchment only. These critical source areas (CSA) are characterized by the occurrence of fast flow processes like surface runoff or macropore flow to tile drains. Moreover, topographic barriers often interrupt the overland flow into the adjacent brook and lead to internal sink areas. From there artificial drains can create a shortcut to the stream network. We tested the predictability of CSA with a modified version of the hydrological Soil Moisture Distribution & Routing model (SMDR). The study area was a small agricultural catchment in Switzerland, in which herbicide losses to surface waters had been experimentally investigated. The small-scale structures, relevant for surface connectivity, were derived using terrain analysis algorithms based on a high-resolution digital elevation map. The analysis showed that surface runoff from a large part (66%) of the study area cannot reach the stream network. Based on prior parameter estimates, the simulated discharge agreed well with the measured values for spring 2000 (Nash-Sutcliffe coefficient of 0.88). Surface saturation was mainly predicted for Gleysol areas, whereby topography was the main driver, and not soil properties. The spatial distribution of CSA and predicted runoff processes agreed well with measured herbicide losses. The main losses were predicted for connected areas prone to surface runoff; additional drained sinks (reinfiltration areas on unconnected areas) were identified as potential risk areas. The predictions are subject to substantial uncertainties. A local sensitivity analysis revealed that the model is most sensitive to parameters describing the lower boundary of the soil (deep percolation and depth of the soil). The spatial extent and the efficiency of the drainage system are also crucial for the spatial variability of herbicide losses.

Keywords: hydrological modelling; critical source areas (CSA); connectivity; SMDR; herbicide losses

2.1 Introduction

The use of herbicides is common practice in modern agriculture. However, part of the herbicides may be transported from the soil to surface and ground waters, where they may affect the ecosystem (Liess and Von der Ohe, 2005) and impair drinking water quality. Therefore, reducing herbicide losses to surface waters is of high practical relevance. Measures to reduce herbicide losses cover a wide spectrum of approaches ranging from the development and use of products that are less harmful to the environment, to substituting chemical by mechanical treatment or the retention of herbicide
losses within buffer strips (e.g. Pätzold et al., 2007).

Since the development of the partial area concept (Betson, 1964) and the notion of variable source areas in the 1960s (Hewlett and Hibbert, 1965), hydrological research has shown that runoff generation is generally restricted to a limited part of a catchment. While these hydrological concepts have been criticized for being overly simplistic (McDonnell, 2003), they still offer a promising concept for managing agricultural areas. Over the last 10 years this concept has been adapted to the management of critical source areas (CSA) for phosphorus (P) losses (e.g. Gburek and Sharpley, 1998; Pionke et al., 2000; Heathwaite et al., 2005; Lazzarotto et al., 2006). The basis for adaptation is the observation that diffuse P losses do not originate from all areas where P is available in excess but only from those where P is actually transported into water bodies. The ability to predict such risk areas would offer options for implementing targeted measures in those areas which generate losses to water bodies.

An important assumption behind the application of the CSA concept to herbicide losses is that the spatial heterogeneity of herbicide losses is dominated by hydrological factors while factors affecting e.g., sorption or degradation rates are less important. Indeed, several studies have demonstrated that factors like topography and hydrological soil properties explain spatial patterns of herbicide losses (Blanchard and Lerch, 2000; Leu et al., 2004b). In many field studies however, it is impossible to trace back observed spatial differences of herbicide losses to field characteristics because of uncertainties about the spatial distribution of herbicide input. One of the exceptions was an intensive field study by Leu et al. (2004a) where the applications of all corn herbicides in a catchment were controlled. The experiment clearly demonstrated that hydrological factors dominated the spatial heterogeneity of losses (Leu et al., 2004b) and factors like sorption properties for mobile substances were less important (Stamm et al., 2004).

These empirical data suggest that the problem of locating CSA is translated into the hydrological problem of predicting areas where fast flow processes to surface waters occur. Since these processes can hardly be directly observed, any such approach has to rely on some sort of spatially distributed hydrological modelling. Many models have been developed over the last years (see e.g. Borah and Bera, 2003) and they have become an important tool for developing land use planning. Nevertheless, their use has not been unchallenged. The available models may lack crucial processes that need to be included in order to properly represent a particular natural system. One of these processes is preferential flow, which is difficult to implement in catchment-scale models. Neglecting this mechanism causes problems in correctly describing infiltration into the soil and in accounting for solute losses to subsurface drains. Another process that is
rarely accounted for is the retention of surface runoff within sink areas. Richards and Brenner (2004) for example observed in a watershed in Michigan that many areas do not generate surface runoff directly reaching the river. They demonstrated that accounting for surface connectivity considerably improved the delineation of risk areas. Leu et al. (2004b) also found that connectivity may be of crucial importance because topographic barriers may prevent surface runoff and hence herbicides to reach the brook. While processes like preferential flow or retention in sink areas may be implicitly accounted for in larger-scale models that are based on e.g., export coefficients (Frink, 1991; Zobrist and Reichert, 2006), they need to be incorporated explicitly into more physically-based models suitable for smaller catchments.

There has also been fundamental critique regarding distributed modelling due to large discrepancies between the data needed to parameterize these models and the data actually available. In many cases, the identifiability of the parameters - due to a lack of data - is so weak that many different parameter combinations may result in equally good fits (Beven, 1993). Accordingly, the physical interpretation of the parameter values is questionable.

The resulting plea for simpler models, which respect the limited data, seems to be at odds with the need of spatially precise predictions that can be used for land use management. A possible way out of this dilemma is the use of hydrological response units defined by e.g., topographic characteristics and soil type. Hydrological soil classes derived from pedological information explain large proportions of the observed spatial variability of the base flow index in conceptual soil type-models (Boorman et al., 1995; Marechal and Holman, 2005; Schneider et al., 2007). This suggests that soil attributes integrate much of the effects of climate, topography and parent material. Hence, the hydrological differences between soil types may be substantially larger than within soil types.

Using different approaches, the work of e.g., Lazzarotto et al. (2006) and Schmocker-Fackel et al. (2007) demonstrated that conceptual models differentiating between pedological soil units are able to characterize small catchments hydrologically and predict the variability within individual catchments. These results suggest that pedological information beyond texture data to feed pedotransfer functions should be used when parameterising spatially distributed or semi-distributed hydrological models. However, the cost for the parsimonious character of these approaches is their conceptual limitation. The HOST approach (Boorman et al., 1995) and the model describing dominant runoff processes (Schmocker-Fackel et al., 2007) for example neglect the spatial topographic position. The soil-type based model of Lazzarotto et al. (2006) makes completely em-
pirical predictions that are based exclusively on discharge data.

In this paper, we suggest combining advantages of physically-based hydrological models with approaches from conceptual soil-type models. We used a distributed physically-based model that treats soil map units as homogeneous but spatially distributed elements in the landscape. In particular, we characterized different soil types by different conditions at their lower boundary. In contrast to many other modelling studies, we focused, apart from discharge, on the quality of spatial predictions of the uncalibrated model. Predicting CSA based entirely on available data, like soil information, topographic data and land use information, makes the model applicable to ungauged catchments, which corresponds to the actual need in practice. This is of high practical importance. In our study, model predictions were tested by comparing the predicted with the measured river discharge. In addition, the measured herbicide losses from three subcatchments of a small agricultural catchment (Leu et al., 2004b) were compared with spatial predictions of generated surface runoff and preferential flow through macropores and artificial drains reaching the channel.

We used the Soil Moisture Distribution and Routing model SMDR (Boll et al., 1998; Frankenberger et al., 1999; Soil and Water Laboratory, 2003; Gerard-Marchant et al., 2006), a fully distributed hydrological model with the objective to identify the location and the spatiotemporal dynamics of areas contributing to fast flow processes. The model accounts for surface runoff and macropore flow. Furthermore, we slightly modified the code to incorporate drainage flow and the effects of sink areas in a simple way. Thus, the modified SMDR included all processes considered relevant based on our previous field experience. In order to understand how spatial predictions may be improved in the future, we investigated which factors caused the spatial heterogeneity of runoff formation and analysed the sensitivity of SMDR towards spatially variable input parameters.

2.2 Methods

2.2.1 Study area

The studied Ror catchment is a small watershed (1.9 km\(^2\)) in the lake Greifensee area near Zurich in the Swiss plateau (Fig. 2.1). Its geologic underground in the northeastern part is formed by tertiary river deposits, the remaining underground consists of moraine material. The topography of the catchment is characterized by moderate
slopes and the area is mainly agriculturally used (90%). A detailed description of the catchment is given in Leu et al. (2004a) and soil properties are discussed in the following section.

![Diagram of catchment with labels](image)

Figure 2.1: a) Location of the Greifensee area within Switzerland b) Location of the Ror catchment in the Greifensee area. c) Aerial photography of the Ror catchment with its subcatchments 1 to 3. Weather stations are displayed by X, the discharge and sampling sites in the brook by circles, the brook by a line (dashed line where it flows in a culvert) and the corn fields of the field study 2000 are shaded (Leu et al., 2004a) (vector25©2006, swissimage©2006 swisstopo, reproduced by permission of swisstopo BA071706).

### 2.2.2 Herbicide and discharge data

Herbicide loss dynamics in the Ror catchment were studied during the growing seasons 1999 (Leu et al., 2005), 2000 (Leu et al., 2004a,b) and 2003 (Gomides Freitas et al., 2008).

In 2000, three herbicides (atrazine, dimethenamid and metolachlor) were applied on several fields in the catchment in a controlled experiment (Fig. 2.1c). This means that the location and the amount of the applied herbicides are known and these herbicides were not used on any other field in the catchment. All treated fields received the same
2.2. Methods

herbicide mixture. Furthermore, all applications were carried out on the same day, so that the herbicides on all fields were exposed to the same weather conditions.

During the weeks following the application (May 5 to August 1), the brooks were intensively monitored at the outlets of three subcatchments (Fig. 2.1c). Discharge was measured and the herbicide concentrations were monitored in flow-proportional high-resolution water samples. In addition, rainfall and air temperature were recorded every 10 minutes at two weather stations in the catchment.

In 1999, discharge and losses of atrazine were measured at the outlet of the catchment (May 23 to September 7). Application data were received from the farmers. Daily rain data were available from a Meteo Swiss station in Grueningen (1.5 km away from the catchment).

Daily potential evaporation rates (pET) were measured at Zurich airport (30 km north-west of the catchment).

2.2.3 Model Description

The SMDR code (Boll et al., 1998; Frankenberger et al., 1999; Soil and Water Laboratory, 2003; Gerard-Marchant et al., 2006) is written in Shell and Perl scripts and directly implemented within the GIS GRASS (Geographic Resources Analysis Support System) Version 5.4 (www.grass.itc.it). The program calculates the water balance without explicit consideration of herbicide transport.

For the implementation, the watershed was divided into multiple layers and each layer into the same number of uniform squares, below referred to as cells. The layers thickness varied according to soil compartment and soil type. The water balance is calculated for constant time steps of 1 day ($\Delta t$). An overview of the relevant processes is given in Fig. 2.2. Water enters the top cells as precipitation and lateral infl ow, $Q_{in}$, from the surrounding upslope cells. It is then routed to the underlying cell by vertical downward flow, $D$, and to the surrounding downslope cells of the same layer by lateral outflow, $Q_{out}$ (top down calculation). Water leaves cells also by root depth dependent evapotranspiration, $ET$. From the lowest cell percolation into a base flow reservoir takes places. At the end of a time step, starting from the bottom cells, any water in excess to the storage capacity of a cell is added to the overlying cell (bottom up). In the top layer the excess water becomes runoff, $E$. The balance for a single cell, $i$, is given by the equation:
Chapter 2. Predicting critical source areas

\[
\frac{\Delta S_{w,i}}{\Delta t} = D_{i-1} + Q_{in,i} - Q_{out,i} - ET_i - D_i - E_i
\]  

(2.1)

where \( S_w \) is the water storage of a cell. \( D_0 \) in the top cell corresponds to the rainfall. The river system in the catchment is not explicitly considered.

In the various SMDR projects slightly different model equations were used. In the following the equations used in our project are briefly discussed (mainly based on Soil and Water Laboratory, 2003).

\[ Q_{aut} = \left( \int_0^z K(\theta) dz \right) W \beta \]  

(2.2)

Figure 2.2: Schematic overview of the water balance representation in SMDR over two soil profiles (m=matrix flow, pf=preferential flow).

**Lateral and vertical flow**

The water flow is calculated as gravity flow described by Darcy’s law but implemented slightly different for vertical and lateral flow. In lateral direction, the flow, \( Q_{out} \) is integrated over the depth \( z \) of a cell whereby the hydraulic gradient is approximated by the local surface slope, \( \beta \).
where \( W \) is the width of a model cell and \( \int K(\theta)dz \) the transmissivity of the cell, with \( K \) being the hydraulic conductivity. In order to calculate the water flow, the volumetric water content, \( \theta \), within a single cell is compared to the macropore drainage limit, \( \theta_{md} \), of the cell. In cells with water contents \( \theta \leq \theta_{md} \) the moisture profile is assumed to be uniform throughout the cell and transmissivity can be integrated directly. Above this limit, the water in the profile is split into a saturated part of depth \( z_{sat} \) in such a way that the water content in the rest of the layer corresponds to the macropore drainage limit \( \theta_{md} \). Preferential flow is taken into account for the saturated part by multiplying the hydraulic conductivity with a depth-dependent factor \( \kappa \) in order to account for the increased conductivity near saturation (Boll et al., 1998). The unsaturated conductivity \( K(\theta) \) is described by an exponential relationship.

\[
\int_0^z Kdz = \begin{cases} 
K_{sat} \left( \exp \left( c \frac{\theta - \theta_{sat}}{\theta_{sat} - \theta_{r}} \right) \right) z & \text{for } \theta \leq \theta_{md} \\
\left( K(\theta_{md}) + (\kappa K_{sat} - K(\theta_{md})) \frac{\theta_{sat} - \theta_{md}}{\theta_{sat} - \theta_{r}} \right) z & \text{for } \theta > \theta_{md}
\end{cases}
(2.3)
\]

where \( K_{sat} \) is the hydraulic conductivity at saturation, \( \theta_{r} \) the residual water content, \( \theta_{sat} \) the water content at saturation and \( c \) an empirical constant with the value of 13 (Steenhuis and Vandermolen, 1986). Lateral outflow \( Q_{out} \) is distributed to the downslope neighbouring cells according to the \( D_{\infty} \) algorithm of Tarboton (1997).

Vertical flow \( D \) is also gravity driven (hydraulic gradient of 1) and calculated by a simplified form of the Richards’ equation, where capillary effects are neglected and the water content is averaged over the cell. The program calculates the potential saturation degree, \( \Theta_{pot} \), which the soil could potentially attain at the end of a time step if drainage was unlimited, as

\[
\Theta_{pot} = 1 - \frac{1}{c} \ln \left( \frac{cK_{sat} \Delta t}{z \Delta \theta} + \exp(c(1 - \Theta_{t-\Delta t})) \right)
(2.4)
\]

where \( \Delta \theta = \theta_{sat} - \theta_{r} \) and \( \Theta = \min \left( 1, \frac{\theta_{sat} - \theta_{r}}{\theta_{sat} - \theta_{r}} \right) \) (derivation in Soil and Water Laboratory, 2003). \( D \) is calculated by the difference between the actual water volume and the calculated potential water content. It is limited by the minimum of the maximal possible downward flow of the actual cell and the cell below according to the saturated hydraulic conductivity with consideration of the macropores multiplier \( \kappa \). At the lower boundary, the hydraulic conductivity of the underlying cell corresponds to the percolation rate. Outflow of the bottom layer of the entire catchment is stored in a lumped linear bedrock reservoir (Frankenberger et al., 1999). The outflow of the reservoir is used to estimate the base flow.
Artificial Drainage

Some areas in the investigated catchment are artificially drained. Such drained areas were not explicitly considered in the available version of the SMDR code (Soil and Water Laboratory, 2003). Based on an idea described in Frankenberger et al. (1999), we changed the program in such a way that all lateral outflow on drained cells is intercepted and directly routed to the outlet of the catchment. Drains are mostly found in flat areas, where the hydraulic gradient in equation 2.2 is small. However, this gradient is artificially increased through drains. Therefore, the hydraulic gradient, derived from the surface slope is not a good approximation for those areas. Instead we estimated an average gradient on drained areas as

$$\beta = \frac{l}{d^2} = E_d$$

where \(l\) is the average water level above the drain, and \(d\) the distance between two drains. Because the model intercepts the flow at the outflow of a cell the slope has to be multiplied with the grid width, \(W\), divided by the drainage space \(d\) to account for the model discretisation.

The quotient \(\frac{l}{d^2}\) is defined as the drainage efficiency \(E_d\). As a simplification, \(E_d\) and hence \(l\), is taken constant over time.

Surface connectivity

In the original code, connectivity and infiltration of surface runoff into downslope cells are not considered and runoff is directly routed to the catchment outlet. To gain a more realistic runoff routing for our study area we divided the watershed into cells that are connected to the river and those that are not. We define connected cells as cells that are, over a continuous sequence of downhill cells, connected with surface water in the catchment. Unconnected cells are further divided into sink cells, where the water accumulates and cells connected to those sink cells. Runoff on connected cells is routed to the river system as in the original code. Runoff on unconnected cells is routed to the associated sink cells. On sink cells, the water is stored and added to the rainfall input on these cells during the next time step. If the surface storage exceeds a storage height of 10 cm, the surplus is routed to the river. The storage height was chosen based on field observation and represents a low value for a topographic barrier.

If the sink cells are artificially drained we additionally allow for a vertical flow component
2.2. Methods

Figure 2.3: Picture of retained surface runoff on agricultural fields in the subcatchment 1 of the Ror catchment (9. 8. 2007) overlaid with a conceptual schema of herbicide losses through the drainage system in sink areas.

into the drain \( (\text{Drain}_{\text{sink}}) \). Water ponding on drained areas may infiltrate into macropores which are directly connected to the drainage system (schema Fig. 2.3). We set the maximum additional drainage term equal to the macropores conductivity of the first layer multiplied with a sink drain efficiency factor \( (M_{\text{sink}}) \):

\[
\text{Drain}_{\text{sink}} = \kappa K_{\text{sat}} M_{\text{sink}}
\]  

(2.6)

As a crude assumption we set \( M_{\text{sink}} \) to 0.1, i.e. about 10 percent of the area is directly connected to the drain by macropores (Shipitalo and Gibbs, 2000; Stamm et al., 2002). The sink areas were identified based on digital elevation models (2 and 25 m resolution) and spatial analysis tools using the following procedure: 1.) fill single pit cells (on the 2 m resolution DEM only, using the Terrain Analysis System (TAS), Lindsay, 2005), 2.) calculate the flow direction and flow accumulation, 3.) determine flow accumulation maxima (= sinks), and 4.) calculate the internal watersheds (IW) of sinks (all within ArcGIS, ESRI, Redlands, USA). IW associated to the river were classified as connected. If there was a topographic barrier between the internal sink and the stream, the IW was classified as unconnected. Finally, the GIS based sink area map was verified in the field. Since we discovered artificial water flow paths which were not reflected in the digital data, we reclassified five IW, as connected.
Evapotranspiration

In SMDR evapotranspiration is calculated as a function of the daily potential evapotranspiration, vegetation condition and the soil moisture according to Thornthwaite and Mather (1955). Basically the ratio between actual to potential $ET$ increases linearly with water content from zero at or below the permanent wilting point, $\theta_{\text{pwp}}$, to a value of one at or above the evapotranspiration limit, $\theta_{\text{etl}}$.

2.2.4 Input data

For the spatial discretisation, the watershed was divided into grid cells with a resolution of 25 m. The resolution is consistent with the available soil map and allows the large number of simulations necessary for uncertainty analysis. The vertical discretisation is based on soil profile description. We implemented 10 layers in our simulation (one A-horizon, one AB-horizon, five different B-horizons, one BC-horizon and one C-horizon). Among the different soil types, between two and seven layers exist. If a layer does not exist, its thickness is set to zero.

Hydrological parameters for all cells are required. To reduce the number of parameters, cells were grouped based on soil units, soil horizons and land cover. In the following sections the necessary input data are described.

Meteorological data: SMDR requires information on rainfall, temperature and potential evapotranspiration. To adjust the initial condition the model was run with an initial warm-up period of three months.

Topography: Two digital elevation models (DEM) with resolutions of 25 m (DHM25©-2003 swisstopo) and 2 m (DTM©2003 swisstopo) were evaluated. The 2 m DEM is based on Airborne-Laser-Scanning with an absolute height accuracy of 0.5 m. The relative accuracy is even better and fine details in the landscape are resolved (see section 2.3.1). For the SMDR simulations, the 2 m DEM was averaged to produce the 25 m grid (Fig. 2.4a).

Soil data: The soil information was derived from a 1:5000 map for agricultural soils (FAL, 1997). The watershed contains a diversity of soil types with various subtypes. Gleysols dominate in flat areas, Cambisols are found on the slopes and some Regosols are present on ridges (Fig. 2.4b). The soil map contains a description of the pedological properties based on reference profiles (16 of them within the Ror watershed). The profile characterisation includes depth, texture, organic matter, and rock content. The depth of the layers, the rock, and gravel content were adopted for model parameterisa-
2.2. Methods

Figure 2.4: Input maps for the SMDR simulation in the Ror catchment: a) elevation (reproduced by permission of swisstopo BA071706), b) soil map, c) land use and d) artificial drainage map. The boundaries of the corn fields of the field study 2000 are delineated and the brook is shown (dotted line where it flows in a culvert).

Based on a soil profile of a Gleysol in the north east of the catchment, analysed during the field study, we replaced a 20 cm thick loam layer with a 50 cm thick sand layer. For the forested area, which is not covered by the soil map, a deep Cambisol was assumed.

Hydraulic soil properties: A number of hydraulic soil properties had to be derived indirectly: The saturated hydraulic conductivity ($K_{sat}$), the residual water content ($\theta_r$),
the water content at saturation ($\theta_{sat}$), the inverse air entry suction $\alpha$, and $N$, a measure of the pore-size distribution were derived using the hierarchical pedotransfer functions of the Rosetta software (Schaap et al., 2001). The water content at field capacity $\theta_{fc}$ (defined by a suction $h$ of -33 kPa) and at the permanent wilting point $\theta_{pwp}$ ($h=-1.5$ MPa) were calculated using the equation of van Genuchten (1980):

$$\frac{\theta_{sat} - \theta_r}{\theta_{sat} - \theta_r} = \frac{1}{(1+|\alpha h|^n)^M} \tag{2.7}$$

with $M = 1 - \frac{1}{N}$

According to Soil and Water Laboratory (2003), the water contents at the evapotranspiration limit, $\theta_{etl}$, was assumed as $0.9 \theta_{fc}$ and at the macropore drainage limit, $\theta_{md}$, as $\theta_{fc}$.

Possible input parameters for Rosetta are texture, bulk density and water retention data. In the soil map only texture data are available. For a more realistic estimation we added estimated bulk density data, which increases with depth. Based on local observation, we set the following densities: for the A-horizon 1.2 g/cm$^3$, for the AB-horizon 1.3 g/cm$^3$, for the B-horizons 1.4 g/cm$^3$, for the BC-horizon 1.5 g/cm$^3$ and for the C-horizon 1.6 g/cm$^3$.

The textures of the soils in the catchment showed variation in the sand and clay fraction, whereas the silt fraction was quite constant ranging mostly between 30 and 40 % (Fig. 2.5). The clay content in Gleysols tended to be higher than in Cambisols. The similar texture results in a relatively uniform distribution of the hydrological parameters for the different soil types. For example, the average of the saturated hydraulic conductivity for the different soils lies between 100 and 200 mm/d, only Regosols have a somewhat higher average (600 mm/d). However, within a soil type the parameter can vary a lot. Gleysols exhibit the largest range (from 40 to 6400 mm/d).

The macropore multiplier $\kappa$, used to correct the hydraulic conductivity for preferential flow, was adopted from Boll et al. (1998). They recommended a multiplier of 10, which decreases exponentially with depth to 1.

**Deep percolation:** The soil map does not contain information about the percolation from the soil profile into the deeper underground. We assumed that the rate of deep percolation that drains the water out of the profile is related to the soil type. As a rough guess we set the percolation in Cambisols to 0.5 mm/day, in Eutric-Gleysols to 0.25 mm/day, and in Gleysols and Regosols (on ridges) to 0. Overall, the average percolation rate was consistent with the average measured base flow and was in the same range as values in other studies (e.g. Evans et al., 1999).
2.2. Methods

Figure 2.5: Textural classes of the different soils in the Ror catchment.

The outflow coefficient of the bedrock reservoir can be estimated from recession curves of the stream hydrographs. On average, base flow receded by 6 % per day.

**Land use:** A land-use map with 25 m resolution was available from Flury et al. (2004) (Fig. 2.4c). The vegetation properties used in SMDR were taken from Gerard-Marchant et al. (2006) supplemented with data on local planting and harvesting dates.

**Artificial drains:** A digital map was available containing all drains in the watershed subsidised by public authorities (Fig. 2.4d). However, this excludes drains installed in an independent, uncontrolled manner by the farmers. For a more realistic representation, we added drains on certain sink areas (see section 2.3.2 for justification). The outflow of some drains occurs outside the catchment. Drain flow from those areas was not considered in the discharge calculation. The mean distance between two drains (d) is 14 m (Leu et al., 2004b) and the water level was initially set to 1 m over the drain and later reduced to 0.25 m (see section 2.3.2).

2.2.5 Quality criterion

The efficiency coefficient of Nash-Sutcliffe (NS) was used to assess the quality of the discharge prediction (Nash and Sutcliffe, 1970):

\[
NS = 1 - \frac{\sum_{t=1}^{T} (Q_o^t - Q_m^t)^2}{\sum_{t=1}^{T} (Q_o^t - Q_o)^2}
\]  

(2.8)
where \( Q_o \) is observed and \( Q_m \) modelled discharge. \( Q^t \) is discharge at time \( t \) and \( \bar{Q} \) the average discharge. The closer the NS coefficient is to one, the better the model prediction.

### 2.2.6 Sensitivity analysis

For sensitivity analysis, SMDR was linked with the software tool UNCSIM (Reichert, 2005). SMDR interacts with UNCSIM through a text file based interface (Reichert, 2006).

In the local sensitivity analysis, a reasonably parameterised simulation was repeated whereby the value of one parameter was slightly changed, while the others were kept constant, to assess how the model output was affected by the change in the parameter.

We considered the local (linear) sensitivity, \( s_i \), of the model results \( y = (y_1, ..., y_n) \) towards the model parameters \( p = (p_1, ..., p_m) \). The sensitivity of the model result \( i \) to the parameter \( j \) is calculated as:

\[
s_{i,j} = \Delta p_j \frac{\partial y_i}{\partial p_j}
\]

where \( \Delta p_j \) is the uncertainty range of model parameter \( j \). The uncertainty range was set equal to the standard deviation. The sensitivity was considered for daily model responses at the outlet of the catchment (discharge) and for the spatially distributed daily surface runoff of all cells in the catchment. To rank model parameters, the sensitivity function over all considered model results \( i \) is calculated as mean square root:

\[
\delta_{j}^{msqr}(p) = \sqrt{\frac{1}{n} \sum_{i=1}^{n} s_{i,j}^2}
\]

For the analysis, model and input parameters have to be supplemented with their uncertainty ranges. Thereby, hydrological parameters for identical soil types and horizons were grouped together to limit computational burden. This results in nine soil types, three horizons (A, B and C) and five hydrological attributes (the van Genuchten parameters \( \theta_{sat}, \theta_r, N \) and \( \alpha \) as well as the saturated hydraulic conductivity \( K_{sat} \)), hence 135 parameters. The variations of these parameters were described as percentage change of the original parameter value.

The uncertainty ranges of the hydraulic parameters reported in the literature vary with texture (Carsel and Parrish, 1988). Since the texture for all soils is similar (compare
Fig. 2.5) and there is no clear correlation between soil type and texture data, we used the same uncertainty ranges for the different soil types. The uncertainty ranges are averages of the standard deviations estimated within Rosetta (Schaap and Leij, 1998) and on the literature values of Carsel and Parrish (1988) (Table 2.1).

### Table 2.1: Averaged uncertainty range of the hydrological parameters

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Parameter</th>
<th>Uncertainty range (%)</th>
<th>Rosetta</th>
<th>Carsel and Parrish (1988)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\theta_{sat}$</td>
<td>saturation water content</td>
<td>5</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>$\theta_r$</td>
<td>residual water content</td>
<td>15</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$N$</td>
<td>measure of the pore-size distribution</td>
<td>100</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>$\alpha$</td>
<td>inverse air entry suction</td>
<td>100</td>
<td>60</td>
<td></td>
</tr>
<tr>
<td>$K_{sat}$</td>
<td>saturated hydraulic conductivity</td>
<td>110</td>
<td>200</td>
<td></td>
</tr>
</tbody>
</table>

The uncertainty ranges of the percolation rates were set to 2 mm/day. Another uncertainty at the lower boundary is the depth of the soil available for water storage since soil can be deeper than the soil profile provided in the soil map. To account for this effect, we added a parameter that potentially increases the soil depth (initial value 0). The uncertainty for the depth was set to 0.5 m.

Finally, the meteorological model input data can include absolute and spatial uncertainties. In our small watershed, we are more concerned about the absolute error and, thus, multiplied the daily data (discharge, temperature and potential evapotranspiration rate) by a constant factor of 20% for the sensitivity analysis.

Uncertainty ranges for all other considered model parameters are listed in Table 2.2.

### Table 2.2: Model parameters with their estimated uncertainty range

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Parameter</th>
<th>Value</th>
<th>Uncertainty range</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_d$</td>
<td>drainage efficiency [-]</td>
<td>$\frac{1}{50}$</td>
<td>0.013</td>
</tr>
<tr>
<td>$M_{sink}$</td>
<td>sink drain efficiency [-]</td>
<td>0.1</td>
<td>0.2</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>conductivity multiplier for the macropores flow [-]</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>$LBC$</td>
<td>linear base flow coefficient [-]</td>
<td>0.06</td>
<td>0.02</td>
</tr>
</tbody>
</table>
2.3 Results

2.3.1 Surface Connectivity

The surface connectivity calculated based on the high-resolution DEM with 2 m resolution indicates that surface runoff from 66% of the catchment cannot directly reach the brook due to local sink areas (Fig. 2.6a). Using a 25 m DEM (Fig. 2.6b) leads to a large underestimation of the unconnected area (only 12%) because information on important topographic features e.g., field roads along the brook, is missing. In general, field observations confirmed the surface connectivity map calculated using the 2 m DEM, but some local corrections were necessary, mainly because of insufficient data on man-made changes of the drainage system.

![Surface Connectivity Maps](image)

Figure 2.6: a) Surface connectivity map of the Ror catchment based on the 2 m resolution DEM and field verification; b) Surface connectivity map based on a 25 m resolution DEM.

2.3.2 Discharge Prediction

A first run of the model relying uniquely on available data without referring to site-specific investigations, showed unrealistic amounts of ponded water on sink areas that were assumed not to be drained based on the available drainage map. The regular occurrence and extent of ponding would render these sink areas too wet for cropping,
which is not the case. Therefore, we assumed these sinks to be drained (except for a wetland area) but relied on the official drainage map for the remaining area. In contrast, the topsoil saturation on fields considered drained was unrealistically low and the drainage efficiency $E_d$ was reduced by a factor of four ($\frac{1}{14}$ to $\frac{1}{56}$, i.e. $l$ from 1 m to 0.25 m).

The simulated discharge with no further parameter adjustments is shown in Fig. 3.3. Due to the coarse temporal resolution of the model the agreement between the simulated and measured discharge can be slightly improved by introducing a lag time into the model. The lag time can be calculated because the measured discharge data are available with a high resolution whereas model results have only daily resolution. The NS-coefficient improved with increasing this lag time up to a maximum of 10 hours, which corresponds to the average response time of measured daily discharge to rainfall. This lag does not correspond to the travel time of the discharge peak. The 5-minutes measurements of rainfall and discharge show only a lag of about 2 hours between rainfall and discharge peak.

In general, the simulated discharge was in reasonable agreement with observations. Using the optimized lag time, the forward prediction had a NS-coefficient of 0.88. Nevertheless, the comparison reveals considerable deviations (Fig 2.8), especially during the large rain event at the end of the period. In most cases, the simulated discharge receded too quickly and the peak discharge was underestimated after dry periods. Thus the variance of the errors increases with increasing discharge (heteroscedasticity).

The transferability of the model parameterisation was checked by simulating the dis-
Chapter 2. Predicting critical source areas

Figure 2.8: Bias analysis for the discharge simulation in the Ror catchment 2000: a) residuals over time b) log-log plot predicted vs. measured discharge.

In qualitative terms the average saturation of the topsoil for the different soil types made sense. The more hydromorphic a soil type was the higher the average simulated degree of saturation. It is interesting to note that, during the larger discharge peaks, Gleysol and Cambisol-Pseudogley were saturated nearly over the whole area. This indicates that runoff was generated on all areas covered by these soils. In contrast, a smaller average degree of saturation was calculated for Cambisols and Regosol.
2.3. Results

![Diagram showing precipitation and discharge](image)

Figure 2.9: Predicted and measured discharge for the Ror catchment during the spring and summer period 1999.

![Diagram showing surface saturation](image)

Figure 2.10: Average surface saturation for the different soils in the Ror catchment during the spring and summer period of 2000; drained areas are not considered.

According to the model structure, topography, soil texture, profile depths and the percolation rate are possible factors causing the different water regime of the different soil types. The influence of topography was assessed by attributing identical properties to all soil types. Even without soil differentiation, the degrees of topsoil saturations for the locations of the different soil types still rank in the order of the hydromorphology of the sites (Fig. 2.11). The average saturation on the sites of Gleysols is higher than on
sites of Cambisols. This implies that topography by itself is an important factor causing spatial differentiation in soil wetness due to lateral water flow even though the relief is not very pronounced in that landscape.

![Hypothetical average surface saturations with an assumed uniform Cambisol profile and percolation for the sites of the different types; drained areas are not considered.](image)

Comparing Fig. 2.10 and 2.11 reveals that the degree of saturation and its temporal development is additionally influenced by texture and percolation rate, which modify the effects of topography.

While these results indicate that the model correctly simulated the spatial differences for the topsoil, the simulated saturation in the lowest layer showed qualitative inconsistencies (data not shown). In contrast to the expectation based on the pedological understanding, the lowest layer of all soil types stayed saturated over the whole period. Such high degrees of saturation is not plausible everywhere and indicates deficits in model structure or parameterization.

2.3.4 Spatial Prediction

The temporal development of the spatial distribution of surface saturation and runoff production was investigated for the first discharge event between May 29 and June 1st 2000 (Fig. 2.12). During this event, the main portion of herbicide was lost (Leu
et al., 2004a). 57 mm of precipitation were measured, the majority falling on the 31st (34.5 mm). The wetness of the soil increased in flat areas along the brook whereas areas on top of a hillslope stayed drier. On May 31, soil saturation as well as surface runoff peaked (Fig. 2.13a). Surface runoff was predicted primarily near the brook. Due to topographic barriers, not all surface runoff ended up in the brook but was retained in internal sinks in the catchment and the connected surface runoff was largely reduced (Fig. 2.13b).

The model predicted saturation and surface runoff also for fields where herbicides were applied in field experiments (Leu et al., 2004a; Stamm et al., 2004) and the measured herbicide losses can be used to test the spatial predictions of the simulated runoff from connected fields and drain flow from sink areas (Fig. 2.14). The comparison was primarily based on losses of dimethenamid because this substance had no significant background concentration. The comparison reveals a very good agreement between the observed herbicide losses and the predicted fast flow volume reaching the brook, that originates from the fields in the three subcatchments on which herbicides were applied (Fig. 2.1c). Connected surface runoff was predicted only for fields in subcatchment 2 (Fig. 2.13b). Preferential flow from sink areas was larger in subcatchment 1 and 2 than in 3. One factor that differentiated strongly between the subcatchments was the surface connectivity. In subcatchment 1 none of the herbicide fields and in subcatchment 3 only a small part of a field is surface-connected to the river network. In contrast three fields in subcatchment 2 are almost entirely surface-connected (compare Fig. 2.6).

### 2.3.5 Sensitivity Analysis

Fig. 2.15 shows the local sensitivity ranking for the simulation of discharge at the catchment outlet and for the spatially distributed runoff during the first discharge event (29th May to 1st June). The parameters are divided into five categories: lower boundary of the soil, meteorological input, drainage system, macropores, and soil hydraulic parameters. Most influential for both objective functions was the percolation rate of the Cambisol, followed by precipitation. In general, the ranking showed that the model results are sensitive to parameters characterising the lower boundary of the soil, mainly the percolation rates and to a lesser extent the depth of the soil. These parameters control the drying of the soil and the available storage capacity before a rain event. Simulations were sensitive to the macropores-conductivity factor $\kappa$ and the drainage efficiency $E_d$, too. There was also some influence of the assumed uncertainty ranges.
Figure 2.12: Calculated surface saturation during the first discharge event after the herbicide application from the 29th of May (top left) to the 1st of June (bottom right) in spring 2000 (saturation in percent). The investigated fields are indicated by white frames, the subcatchment boundaries by dashed lines and the brook by a continuous line (dotted where it flows in a culvert).

Using ranges from Rosetta, the hydraulic van Genuchten parameters \( N \) are quite important whereas \( \alpha \) and \( K_{sat} \) are less important. Using the Carsel and Parrish (1988) uncertainty ranges (data not shown) the model results are more sensitive to \( K_{sat} \) and much less to \( N \). The effect of \( E_d \) can also be demonstrated by the runoff processes on the agriculture fields. A fourfold \( E_d \) leads to a quite different prediction of the runoff.
2.3. Results

a) runoff

[Map of runoff]

500 m

b) connected runoff

[Map of connected runoff]

mm/day

Figure 2.13: a) Calculated surface runoff in the Ror catchment; b) calculated surface runoff for connected areas (plus overflow in the sink areas). Both at the 31st of May. The investigated fields are indicated by white frames, the subcatchment boundaries by dashed lines and the brook by a continuous line (dotted where it flows in a culvert).

processes (Fig. 2.14). Saturation on the drained fields in the subcatchment 1 is largely reduced and as a result also the predicted surface runoff into sink areas. Without the additionally implemented drains on sink areas, the surface runoff in subcatchment 3 is overestimated due to overflow of the sink areas. These effects were already detected during the first plausibility check of the results causing an adaptation of $E_d$ and the drainage map (see section 2.3.2).

The sensitivity ranking further demonstrates that the results are sensitive to parameters for soil types with a high coverage in the catchment (Cambisol, Eutric-Gleysol and Gleysol). Since the distribution of herbicide application may not be equal on all soil types in the catchment, it is interesting to investigate the sensitivity of simulation results to parameters of less frequent soil classes by inversely weighting soil-specific parameters by their fraction in the catchment. Doing so identifies the weighted efficiency of sink drain and the weighted percolation rates of Dystric Cambisol, Cambisol-Pseudogley, and Regosol as most sensitive parameters (data not shown).
Chapter 2. Predicting critical source areas

2.4 Discussion

2.4.1 Relevance of surface connectivity

Our investigation demonstrates the importance of surface connectivity for the prediction of risk areas for diffusive herbicide losses. Because surface runoff is a major transport process, it is crucial for surface water quality whether substances in surface runoff reach the brook or are trapped in internal sink areas. We found that large parts of the catchment are not surface-connected hence surface runoff originating from these areas can not directly reach the brook (Fig. 2.6). Comparisons with other catchments in the larger Greifensee watershed suggest that this is not unusual for this type of landscape. The surface connectivity pattern explained a substantial part of the spatial variability of herbicide losses with the highest herbicide losses being observed on the fields in subcatchment 2. According to our simulations, these were the only fields that contributed significantly to surface runoff entering the brook.

The amount of surface runoff reaching the brook may be largely overestimated if the topographical analysis is based on a DEM with an inadequate resolution. The surface analysis with two DEMs with different resolution (2 and 25 m) demonstrated that the coarser data largely overestimates connected areas because sinks are overlooked. For
2.4. Discussion

Figure 2.15: Ranked model sensitivity to parameters (in %) with regard to discharge (left) and runoff produced on all cells (right) for the Ror catchment (average uncertainties ranges for the soil hydraulic parameters based on Rosetta). N, α: van Genuchten parameters.

Many countries, high-quality DEMs are now becoming available and hence allow good surface connectivity estimations. However, it needs to be mentioned that many GIS routines assume that sinks in a DEM are equivalent to errors and they are removed to carry out hydrological surface analyses. This is inadequate for some areas and purposes, as it has been demonstrated here or by e.g., Richards and Brenner (2004).

On the other hand, the measured herbicide losses demonstrated that there are also losses from unconnected areas via the subsurface drainage system (Leu et al., 2004a). The drainage system is considered the second important flow path for diffuse losses (for example Kladivko et al., 2001) due to preferential flow that quickly by-passes much of the sorbing soil matrix (Stamm et al., 2002). This process is strongly enhanced on ponded sink areas (Fig. 2.3) because preferential flow paths need sufficient lateral inflow to convey large amounts of water and solutes (Flühler et al., 1996; Weiler and Naef, 2003).

Whether sink areas are critical for surface water quality depends on the presence of artificial drains. However, if they are absent sink areas may act as hot spots for local groundwater recharge and pollution. Such effects have for example been observed with frost-induced runoff (Derby and Knighton, 1997). Therefore sink areas are not per se 'no risk areas'. However, herbicide losses to surface waters through subsurface drains
are usually lower than in surface runoff (Kladivko et al., 2001).

Without consideration of surface connectivity, the discharge is still acceptably reproduced but the calculated runoff processes do not correspond to the observed herbicide losses and the field experience.

2.4.2 A priori predictions: potentials and limitations

Overall, the predicted spatial variability of fast-flow generation relevant for herbicide transport agreed very well with the observed losses from the three subcatchments (Fig. 2.14). On the one hand, the successful predictions were due to the correct assessment of surface connectivity using a high-resolution DEM. Without considering surface connectivity (or a surface connectivity calculated based on a coarser DEM) the connected surface runoff on the herbicide fields in subcatchment 1 would be overestimated. On the other hand, the simulated water regimes of the different soil types indicate that the model correctly reproduced important aspects of topsoil hydrology. The results demonstrate that even gentle topography plays an important role in differentiating between soil types, i.e. that saturation is more frequent in certain soils (e.g. in Gleysols) because of their location and their properties. Hence, the water regime is an interplay between relief, texture, lower boundary of the soils and soil depth.

The relevance of boundary conditions was emphasised by the local sensitivity analysis. In contrast to what might be expected, the soil hydraulic properties were not the most influential parameters. Instead, the parameters affecting the lower boundary conditions and the boundary conditions imposed by artificial drainage systems exerted the largest influence given their large uncertainty bands. It fits into this picture that the drainage efficiency was the only parameter we had to adapt after a first plausibility check of the simulations with the uncalibrated model.

The calculated sensitivity ranking is dependent on the uncertainty ranges. The used uncertainty estimates for the van Genuchten parameter were compared with data from Carsel and Parrish (1988) (Table 2.1). In both cases, the estimated uncertainty ranges are quite large but there is considerable variation between the estimates from the two sources, which leads to a different ranking among the parameters.

The results of the sensitivity analysis cannot be discussed without referring to the temporal resolution of the SMDR model. Using a constant time step of one day implies that the average daily rain intensities did not exceed the estimated hydraulic conductivities of the different soils in the catchment. A comparison with the measured 5-min rainfall data revealed that even these hardly ever exceeded the conductivity values (data not
shown) and if so, Hortonian overland flow may have occurred for very short periods only. Nevertheless, it can be expected that the soil hydraulic properties would gain importance in a sensitivity analysis based on a model and input data with a high temporal resolution.

A further aspect related to the temporal resolution warrants a short discussion. We found that a time lag had to be introduced into the model for an optimal agreement. An analysis of the measured rain and discharge showed that the time lag can be explained by the mean response time of the catchment. There may be an additional effect of the average rainfall distributed during a day. Since the average duration of discharge peaks as well as the actual lag between rainfall and discharge peak are clearly less than one day, the daily resolution leads to a loss of information.

The high saturation in the bottom layer and the model mismatch during the hydrograph recessions indicate further options for model improvement. Both results may be due to the hydrologic gradients that are assumed to be constant in time. It would be interesting, also from the conceptional point, to make the gradient dependent on the water content.

### 2.5 Conclusion

Our results highlight hydrological modelling as a powerful tool in the prediction of CSA for diffuse herbicide losses. Entirely based on data that are generally available or become available in many regions in the foreseeable future (high-resolution DEMs) and with the adjustment of a few parameters without prior information, it was possible to predict the large spatial heterogeneity of herbicide losses observed in the field experiment. The identification of risk areas is not limited to herbicides but can also readily be extended to other diffuse pollutants triggered by hydrological processes.

While many papers on hydrologic modelling put a main emphasis on parameterising the soil hydrological properties correctly, our results indicate that a proper assessment of the lower boundary conditions including their spatial distribution is of critical importance. This result is expected to hold for conditions where runoff generation is mainly caused by saturation excess and to a lesser degree by Hortonian runoff.

Assessing the effects of surface connectivity with high-resolution DEMs seems necessary in intensively farmed landscapes of moderate topography, which may be additionally affected by man-made modifications of the relief. Neglecting internal sink areas may strongly over-estimate the contribution of surface runoff in such areas. On the other hand, sink areas may be hot spots for preferential flow. In the presence of arti-
facial drains, this may imply substantial losses to surface waters, in their absence, the sinks may cause localized groundwater pollution. The complexity of these topographical and pedological effects on diffuse herbicide pollution emphasises the usefulness of distributed hydrological models in the delineation of CSA and catchment-scale risk assessments.

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Bibliography


Chapter 3

Reduction of structural uncertainties in hydrological modeling using discharge data in a Bayesian Inference approach

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submitted to Water Resources Research
Abstract  We used a spatially distributed hydrological model (a modified version of the Soil Moisture Distribution and Routing model SMDR) to simulate the spatial distribution of saturated areas with the goal to identify risk areas for diffuse pollution in a small agricultural catchment in Switzerland. Given the available data, knowledge of the model parameters is coarse and thus prior predictions involve large uncertainties. We investigated to which degree river discharge data can confine parameter values and decrease the uncertainty in the spatial prediction. Thereby, we combined the prior knowledge with additional river discharge data to overcome the problem of model parameter identification within a Bayesian inference approach. To consider the effect of uncertainty in input data and model structure we formulated the likelihood function with an autoregressive error model additive to the river discharge calculated by the deterministic hydrological model. Due to the additional information of the discharge the width of some of the marginal parameter distributions could be reduced, which largely decreased the uncertainty of the spatial prediction. The applied error model helped to fulfill the statistical assumptions of the inference process. However, the model structure remained critical. Differences in the discharge prediction pointed to deficits in the implementation of the lower boundary conditions of the soil profile. With improvements in the model structure we were able to significantly reduce the model structure bias and thus improve the statistical basis of the probabilistic prediction. Furthermore, the improved model structure decreased the spatial prediction uncertainty.

Keywords: hydrological modeling; Bayesian inference; model structure deficits; bias

3.1 Introduction

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 such as herbicides. It has been demonstrated that such losses are strongly related to the hydrology of a catchment, and that the primary losses are limited to areas in a catchment which are prone to 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 areas where mobile nutrients or pesticides are available for transport, they are called critical source area (CSA). The delineation of CSA is crucial for effective mitigation of surface
water contamination.

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 in an appropriate resolution. Model input has to be estimated from generally available data like soil maps or land use data, which are often coarse and lead to quite 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 intensively discussed, but until now no generally accepted method to address all the different sources of uncertainty has been established (compare discussion Mantovan and Todini, 2006; Beven et al., 2008). Interesting methods to estimate uncertainty intervals 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) or multiple criteria approaches (Gupta et al., 1998; Vrugt et al., 2003b).

For a practical implementation of mitigation and management strategies, it is crucial first to reduce the uncertainties as much as possible and secondly to correctly communicate the uncertainties to stakeholders. An obvious choice to reduce uncertainty is to search for additional information which has not been used to formulate and parameterize the model. In many cases, river 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). Since mechanistic hydrological models typically have many spatially distributed parameters, the achievable reduction in parameter uncertainty is likely limited. In order to examine to what extent this is the case, we combined prior information with measured data by Bayesian inference. In Bayesian statistics, probability distributions are used to describe the knowledge or belief of the analyst. When applying these techniques in environmental decision support, it is the analyst’s objective to describe defendable, intersubjective current scientific knowledge, rather than his or her subjective beliefs. Prior knowledge about the model structure is described by the likelihood function of the model, the probability density of model results given the parameters. 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 (Kennedy and
Chapter 3. Uncertainty analysis

O'Hagan, 2001; O'Hagan, 2003). This updating procedure is usually implemented by a Markov Chain Monte Carlo (MCMC) algorithm. This has been previously done with hydrological models (for example Kavetski et al., 2006b; Yang et al., 2007; Huard and Mailhot, 2008). However, even when combining additional measured data with prior information, there may still be relatively large volumes in parameter space that contain parameters that lead to similar results (parameter non-uniqueness). In a Bayesian context it results naturally when the posterior is fat in certain directions (it will not be as fat as when using some "generalized" likelihood functions as it is done in some GLUE applications).

In order 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 defendable, intersubjective belief about the outcome of random processes, we can combine frequentist and Bayesian elements when formulating a likelihood function of a system that contains random elements. The effect of (random) input errors and stochastic errors in the model structure lead to autocorrelated errors in model output. If we add an independent observation error, we still end up with an autocorrelated error model that has a frequentist interpretation. Despite updating our knowledge of model parameters in a Bayesian framework, we were thus able to apply frequentist tests to the residuals to analyze for systematic errors of the deterministic model. We will show that we can reduce these systematic errors by reducing structural deficits of the model.

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). In Frey et al. (2009) we showed - based on a priori estimated parameters - that the simulated discharge in our study catchment for the spring and summer of 2000 agrees well with the measured data. However, the residual analysis showed systematic deviations between measured and simulated discharge values. In particular, in the recession parts of the hydrograph after flood events, the predicted discharge declined too fast and the base flow in dry periods was overestimated. The predicted spatial distribution of fast transport processes matched the observed herbicide losses from three different subcatchments very closely. Thereby the consideration of the surface connectivity was crucial.

The objective of this work was to analyze the uncertainty in CSA prediction and to which degree it can be reduced using river discharge data within a particular case study. First, we quantified the uncertainty of the prior prediction described in Frey et al. (2009). This
was done by extending the best guess model parameters to prior probability distributions and propagating these through the deterministic model. This was implemented numerically by a Monte Carlo simulation. The second objective consisted of investigating to which degree the prediction uncertainty can be reduced by using measured discharge to constrain the model parameters. Therefore, it is 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 affect the spatial prediction of saturated areas in the catchment.

3.2 Methods

3.2.1 Study area and calibration data

The study site is a small agricultural catchment of 1.9 km\(^2\) within the Swiss plateau (Fig. 3.1). It has a moderate topography, the elevation ranges from 490 to 550 meter above sea level, and the annual precipitation averages 1330 mm. Details can be found in Leu et al. (2004a) and Frey et al. (2009).

During three growing seasons, herbicide losses in different parts of the catchment were monitored. Here, we focus on a controlled herbicide application in the year 2000 (Leu et al., 2004a,b). All corn fields in the catchment - but not any other field - received the same herbicide mixture (including atrazine, dimethenamide and metolachlor) during the same day. In the weeks following the application (May 5 to August 1) the stream was intensively monitored at the outlets of three subcatchments (Fig. 3.1). Discharge and herbicide concentrations were measured at three sites. Furthermore, two weather stations in the catchment recorded rainfall and air temperature. We used this data for model calibration and validation.

3.2.2 Model

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 (Frankenberger et al., 1999; Soil and Water Laboratory, 2003; Gerard-Marchant et al., 2006). The code of SMDR is implemented in the GIS environment
Figure 3.1: Aerial picture of the study catchment with its three subcatchments and its position within Switzerland, the corn fields of the study campaign 2000 are shaded (Leu et al., 2004a). (Swissimage, vector25 ©2003, reproduced with the permission of swisstopo, JA082266)

GRASS (www.grass.itc.it).

The catchment is divided horizontally into uniform squares (= soil columns) with multiple vertical layers (Fig. 3.2). 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. Infiltration excess runoff can also occur if the rain input exceeds the hydraulic conductivity of the first layer. The lateral and vertical water flow between model cells is calculated based on 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 with a minimum gradient in flat areas. If a soil is artificially drained the hydraulic gradient is approximated by a mean hydraulic gradient (the drainage efficiency coefficient $E_d$). The hydrological conductivity is described by an exponential relationship of 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 $\kappa$, 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).
Evapotranspiration is calculated based on the measured daily potential evapotranspiration, the growth of the vegetation condition and the actual soil moisture (Thornthwaite and Mather, 1955). From the bottom cell the water percolates into a base flow reservoir. Thereby, the water flow is limited by a percolation rate, \( \text{per} \), which is constant over time but varies in space with the soil type. Base flow is calculated as outflow of the reservoir with a constant coefficient, \( LBC \). At the end of the constant daily time step, all water in excess to the water storage capacity of the soil column is converted into overland flow.

To adapt the program to the local conditions, we added two additional processes. First, we accounted for artificial tile drains as mentioned above: Lateral flow on drained areas is directly routed to the river system (idea adapted from Frankenberger et al., 1999). Second, we considered the connectivity to the stream: In the released version of SMDR (Soil and Water Laboratory, 2003) all surface runoff is directly routed to the catchment outlet assuming that all areas are on the surface connected to the river system. Analysis of a high-resolution DEM (digital elevation model) combined with field observation showed that this is not the case for large parts of our study catchment. Therefore, we implemented a process which considered the re-infiltiration of surface runoff accumulating in sink areas. If the sink areas were artificially drained, the model allowed for an additional direct drainage flow to the river system. The amount of water that is transferred to the river in one time step depends on the sink drain efficiency parameter, \( M_{sink} \) (Frey et al., 2009). In the remaining part of the article we will refer to this model as “original”.

Figure 3.2: Conceptual overview of the water fluxes considered in a soil column in the SMDR model.
3.2.3 Improvements of the model structure

As it will be discussed in section 3.3.2 and 3.4.1, the original model led to systematic deviations between calculated and measured river discharge during dry weather conditions. To improve the model the constant percolation rate was replaced by dynamic percolation rate \( \text{per} \) that changes with the height of the water table, \( h \), by introducing a soil-specific factor \( f_{\text{soil}} \):

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

(3.1)

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, \( f_{\text{lat}} \):

\[
\beta_{\text{drained}} = h \cdot E_d \cdot f_{\text{lat}}
\]  

(3.2)

It is possible that there is some exchange of groundwater across the catchment boundaries defined by surface topography. Therefore, we introduced 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:

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

(3.3)

Furthermore, since one run of the model lasted too long for obtaining a sufficient number of simulations needed for a statistical analysis, we had to rewrite the water balance calculation part of the modified model, which was coded in GRASS, in a faster language (FORTRAN 95).

3.2.4 Prior Parameter Estimates

For parameterization, the SMDR model requires spatially distributed information about topography, land use, and soil types. This spatially distributed information has to be combined with parameters describing the properties of the different soil and land use classes. In addition, some general parameters (such as drainage efficiency or macropore coefficients) are required. Best guess values for these parameters were derived
from the literature, other modeling studies, and expert knowledge as described in Frey et al. (2009).

The prior values for the hydrological parameters (Table 3.1) were calculated by pedo-transfer 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, \( N \), the inverse air entry suction, \( \alpha \), and the saturated hydrological connectivity, \( K_{sat} \), were relevant (van Genuchten, 1980).

In order to limit the number of 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 in Kavetski et al., 2006a,b; 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 3.1). 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 (basis local sensitivity analysis in Frey et al., 2009). These were the parameters in the A-horizon of the forest, Cambisol, Eutric-Gleysol and Gleysol, in the B-horizon of Cambisol, and in the C-horizon of Cambisol and forest.

Since prior information for general parameters and the percolation rates was vague, wide distributions were chosen (Table 3.2 and Table 3.3). All parameters were assumed to be independent and their joint prior probability density was equal to the product of their marginal densities.

According to Frey et al. (2009) 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 is relatively low, we assumed input uncertainty to be small and did not consider this type of uncertainty.

### 3.2.5 Uncertainty analysis of prior prediction

Frey et al. (2009) carried out a prior simulation with the parameter values labeled “mean” in Tables 3.1 to 3.3. 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).
Table 3.1: Marginal prior distributions of the multipliers of the hydrological parameters. This set of multipliers exists for every soil type and layer, but the distribution for all parameters are assumed to be equal. The normal and lognormal distributions are truncated at “min” and “max”; “mean” and “standard deviation” refer to the means and standard deviations of the non-truncated distributions.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Distribution</th>
<th>Mean</th>
<th>Standard deviation</th>
<th>min</th>
<th>max</th>
</tr>
</thead>
<tbody>
<tr>
<td>saturation water content (as relative deviation) [-]</td>
<td>$\theta_{sat}$</td>
<td>normal</td>
<td>1</td>
<td>0.25</td>
<td>0.5</td>
<td>2</td>
</tr>
<tr>
<td>residual water content (as relative deviation) [-]</td>
<td>$\theta_r$</td>
<td>normal</td>
<td>1</td>
<td>0.3</td>
<td>0.1</td>
<td>2</td>
</tr>
<tr>
<td>measure of the pore-size distribution (as relative deviation) [-]</td>
<td>$N$</td>
<td>normal</td>
<td>1</td>
<td>0.2</td>
<td>0.08</td>
<td>5</td>
</tr>
<tr>
<td>inverse air entry suction (as relative deviation) [-]</td>
<td>$\alpha$</td>
<td>lognormal</td>
<td>1</td>
<td>0.35</td>
<td>0.1</td>
<td>10</td>
</tr>
<tr>
<td>saturated hydraulic conductivity (as relative deviation) [-]</td>
<td>$K_{sat}$</td>
<td>lognormal</td>
<td>1</td>
<td>1.2</td>
<td>0.01</td>
<td>100</td>
</tr>
</tbody>
</table>

3.2.6 Bayesian Inference

In order to obtain information on how the parameter distributions change when using additional data, we evaluated the posterior distributions of parameters given the data $p(\theta \mid y^{obs})$ using the theorem of Bayes (Gelman et al., 1995):

$$p(\theta \mid y^{obs}) = \frac{p(y^{obs} \mid \theta)p(\theta)}{\int p(y^{obs} \mid \theta')p(\theta') \delta \theta'}$$ (3.4)

where $p(\theta)$ is the prior probability density of parameters and $p(y \mid \theta)$ is the likelihood function of the model, i.e. the probability density of model results, $y$, given the parameters. The likelihood function of the model describes prior knowledge about the model structure and can still have a frequentist interpretation, as frequentist probabilities can be used as defendable beliefs about the outcome of a system, if random elements dominate the uncertainty.

The deterministic model is a function of model parameters, $\theta$, and the structure of the deterministic part of 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 $t_i$: 
3.2. Methods

Table 3.2: Marginal prior distributions of general model parameters. The normal and lognormal distributions are truncated at “min” and “max”; “mean” and “standard deviation” refer to the means and standard deviations of the not truncated distributions. Parameters with ⋆ are only investigated in the calibration of the original version, parameters with † only in the improved model structure.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Distribution</th>
<th>Mean</th>
<th>Standard deviation</th>
<th>min</th>
<th>max</th>
</tr>
</thead>
<tbody>
<tr>
<td>drainage efficiency [-]</td>
<td>$E_d$</td>
<td>transformed normal $^\dagger$</td>
<td>28</td>
<td>10</td>
<td></td>
<td></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>

$^\dagger$ due to model constraints the sample for $E_d$ was drawn from an underlying normal distribution of $d$ ($E_d = d^2$). Their mean, $\mu_d$, and standard deviation $\sigma_d$ are given in the table. The probability density of $E_d$ is then given by:

$$f(E_d) = \frac{1}{\sigma_d \sqrt{2\pi}} \exp \left( -\frac{1}{2} \left( \frac{E_d - \mu_d}{\sigma_d} \right)^2 \right)$$

$y^M(\theta) = (y^M(\theta)_t_0, y^M(\theta)_t_1, \ldots, y^M(\theta)_t_n)^T$ (3.5)

Deviations between the simulation results of this deterministic model and measured data are due to measurement errors in output observations, due to errors in input, initial and boundary conditions, and due to errors in model structure. We cannot assume the output 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 carry out a Box-Cox transformation (Box and Cox, 1964, 1982) as done in Schuwirth et al. (2008) and Yang et al. (2007) and rewrite the probabilistic output of the model as the vector of random variables

$$Y_{t_i}^M = g^{-1}(g(y_{t_i}^M) + E_{t_i}))$$ (3.6)

where $E_{t_i}$ is the error term in transformed units and $g$ and $g^{-1}$ are forward and backward Box-Cox transformations given by
Table 3.3: Marginal prior distributions of the percolation rates and the percolation factors for the modified model structure. The normal distributions are truncated at “min” and “max”; “mean” and “standard deviation” refer to the means and standard deviations of the not truncated distributions. Parameters with ⋆ are only investigated in the calibration of the original version, parameters with † only in the improved model structure.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Parameter</th>
<th>Distribution</th>
<th>Mean</th>
<th>Standard deviation</th>
<th>min</th>
<th>max</th>
</tr>
</thead>
<tbody>
<tr>
<td>percolation Cambisol [mm/day]</td>
<td>perCam ⋆</td>
<td>normal</td>
<td>0.5</td>
<td>2</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>percolation Calcareous Cambisol [mm/day]</td>
<td>perCaC ⋆</td>
<td>normal</td>
<td>0.5</td>
<td>2</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>percolation Dystric Cambisol [mm/day]</td>
<td>perDyC ⋆</td>
<td>normal</td>
<td>0.5</td>
<td>2</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>percolation Cambisol-Pseudogley [mm/day]</td>
<td>perCaP ⋆</td>
<td>normal</td>
<td>0.25</td>
<td>2</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>percolation Eutric-Gleysol [mm/day]</td>
<td>perEuG ⋆</td>
<td>normal</td>
<td>0.25</td>
<td>2</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>percolation Gleysol [mm/day]</td>
<td>perGle ⋆</td>
<td>normal</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>percolation Wet Gleysol [mm/day]</td>
<td>perWeG ⋆</td>
<td>normal</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>percolation Regosol [mm/day]</td>
<td>perReg ⋆</td>
<td>normal</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>percolation forest [mm/day]</td>
<td>perfor ⋆</td>
<td>normal</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>factor Cambisol [1/day]</td>
<td>fCam †</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/day]</td>
<td>fCaC †</td>
<td>normal</td>
<td>0.45</td>
<td>1.8</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>factor Dystric Cambisol [1/day]</td>
<td>fDyC †</td>
<td>normal</td>
<td>0.45</td>
<td>1.8</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>factor Cambisol-Pseudogley [1/day]</td>
<td>fCaP †</td>
<td>normal</td>
<td>0.225</td>
<td>1.8</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>factor Eutric-Gleysol [1/day]</td>
<td>fEuG †</td>
<td>normal</td>
<td>0.225</td>
<td>1.8</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>factor Gleysol [1/day]</td>
<td>fGle †</td>
<td>normal</td>
<td>0</td>
<td>1.8</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>factor Wet Gleysol [1/day]</td>
<td>fWeG †</td>
<td>normal</td>
<td>0</td>
<td>1.8</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>factor Regosol [1/day]</td>
<td>fReg †</td>
<td>normal</td>
<td>0</td>
<td>1.8</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>factor forest [1/day]</td>
<td>for †</td>
<td>normal</td>
<td>0.45</td>
<td>1.8</td>
<td>0</td>
<td>10</td>
</tr>
</tbody>
</table>

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

\[
g^{-1}(z) = \begin{cases} 
\lambda_0 \cdot (\lambda_1 z + 1)^{1/\lambda_1} - \lambda_2 & \text{for } \lambda_1 \neq 0 \\
\lambda_0 \exp(z) - \lambda_2 & \text{for } \lambda_1 = 0 
\end{cases}
\]

Here, \( Y^M \) is the vector of random variables representing the model result, \( y^M \), including the stochastic errors. The parameters \( \lambda_1 \) and \( \lambda_2 \) are used to reduce heteroscedasticity and to make the error term \( E_t \) approximately normally distributed. \( \lambda_0 \) was implemented to make the expression in the paranthesis dimensionless. It has a value of 1 and the same units as the model result. To test the statistical assumption of the normal distri-
bution of the error we analyze the standardized residuals, $r$, of transformed data and model results.

$$ r = \frac{g(y_{obs}^t) - g(y^M(\theta))}{\sigma} $$

(3.8)

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

To account for the autocorrelation of the residuals we apply a time continuous autoregressive error model (Yang et al., 2007). It is assumed that the innovations, $I_t$, rather then the residuals are independent

$$ I_t = E_t - E_{t-1} \exp \left( -\frac{t - t_{i-1}}{\tau} \right) $$

(3.9)

and normally distributed with a standard deviation of

$$ \sigma_I = \sigma \sqrt{1 - \exp(-2\frac{t - t_{i-1}}{\tau})} $$

(3.10)

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

We can expect the errors to be strongly autocorrelated in the recession part of the hydrograph, but only weakly during rain events. We therefore use 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 exceeds 1.5 mm/day $\tau$ was reset to 1 day. To test the assumption of independency of the innovations we compare the standardized observed innovations of the transformed data and the transformed model results:

$$ I_t = \frac{g(y_{obs}^t) - g(y^M(\theta)) - (g(y_{obs}^{t-1}) - g(y^M(t_{i-1})(\theta))) \exp(-\frac{t - t_{i-1}}{\tau})}{\sigma \sqrt{1 - \exp(-2\frac{t - t_{i-1}}{\tau})}} $$

(3.11)

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

Combining the deterministic model with the Box-Cox transformation and the autoregressive error model leads to the following likelihood function (Yang et al., 2007):

$$ p(y_{obs} \mid \theta) = \frac{1}{\sqrt{2\pi}\sigma} \exp \left( -\frac{1}{2} \left[ \frac{g(y_{obs}^t) - g(y^M(\theta))}{\sigma^2} \right]^2 \right) \left| \frac{dg}{dy} \right|_{y=y_{obs}^t} $$
Numerically, a sample from the posterior distribution (equation 3.4) was derived by applying the Metropolis-Hastings Markov Chain Monte Carlo (MCMC) algorithm (Gelman et al., 1995) using UNCSIM. To avoid a burn-in, first a parameter optimization to maximize the likelihood was carried out. We used the algorithm SCE-UA (Duan et al., 1993) implemented in UNCSIM. Starting from the best estimates of the parameter values, the MCMC chains were started. In an iterative procedure, the initial runs were used to update the proposal distribution to ensure an efficient sampling. Furthermore, for the improved model multiple chains were calculated to compare their convergence.

3.3 Results

3.3.1 Uncertainties in discharge prediction

The uncertainty range of the a priori prediction does not always capture the measured data (Fig. 3.3a). Particularly the base flow is overestimated. 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. For the prior prediction, some percolation rates, for example for Gleysoils and Regosols, were set to 0. The corresponding prior marginal is a normal distribution with mean 0 truncated at zero. This truncation shifts the mean from zero to a positive value and causes a poorer fit.

In contrast to the prior simulation, the 90% uncertainty interval of the original model calibrated with discharge data (Fig. 3.3b) 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 the model structure. Furthermore, the maximum and the median of posterior density are in good agreement. They have Nash-Sutcliffe coefficients of 0.90,
3.3. Results

Figure 3.3: Comparison of the measured and the simulated discharge, including 90% prediction uncertainty band, for the study catchment during the spring period 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 are calculated at every time step and the maximum posterior probability density is determined for the whole calibration period.
which is slightly higher than in the prior simulation. However, the base flow remains overestimated.

Improvements in the model structure mainly alter the recession and the base flow portion of the hydrograph as expected (Fig. 3.3c). Despite a narrower uncertainty band it nearly always covers the measured values. This indicates a reduction in the model-structural error. This conclusion is supported by the fact that the parameter set with the maximum posterior density has a Nash-Sutcliffe coefficient of 0.92 exceeding all other values.

### 3.3.2 Residual analysis of the predictions of the calibrated models

The residuals and innovations of measured data and maximum posterior model results are analyzed to test the statistical assumption (normally distributed and independent innovations) underlying the likelihood function (Fig. 3.4). Note that our likelihood function has a frequentist interpretation despite doing Bayesian inference (see section 3.2.6).

Comparing the normalized residuals of the original model before and after Box-Cox transformation (Fig. 3.4a) demonstrates a reduced heteroscedasticity and a more homogenous distribution of the variance after Box-Cox transformation using transformation constants $\lambda_1 = 0.3$, and $\lambda_2 = 0.05$ mm/day. In Figure 3.4c, the normalized residuals (above) and the innovations (below) of the original model are plotted over time. The normalized errors are strongly autocorrelated. Negative residuals are mostly followed by another negative value and positive residuals by another positive value. In contrast, the sequence of innovations of the error model shows much more variation and demonstrates the usefulness of the error model. During two dry periods (beginning and middle of the calibration period), however, the innovations still show strong autocorrelation. Furthermore, the normalized residuals at low measured discharge are predominately negative (Fig. 3.4c). These observations correspond to the overpredicted discharge during low-flow periods using the original model.

The improvements in the model structure led to a much more balanced variance at low discharge (Fig. 3.4b) and a reduced autocorrelation during dry periods (the sign of the innovations in Fig. 3.4d has more random variation). The improvements resulted in a higher nonlinearity of the model response and an improved agreement between the statistical assumptions and the distribution of residuals and innovations.
3.3.3 Restriction of the parameter space

By comparing prior and posterior marginal probability densities we analyzed how much the parameter space can be restricted through the calibration data (Fig. 3.5 and 3.6). As indicated by reduced widths of the posterior marginals, for the original model, knowledge was gained primarily for parameters $N$ and partially for $K_{sat}$ and for most of the parameters of the improved model. No large shift of the distribution maxima occurred with the exception of the multipliers of $K_{sat}$. For $M_{sink}$, the calibration could largely reduce the uncertainty range but little prior information was available anyway. In the improved model, $M_{sink}$ was estimated clearly higher than in the original model. The macropore parameter $\kappa$ in the original model tends to be somewhat higher than in the reference study of Boll et al. (1998) but overall it remains in the same range. The reduction of the relatively high prior uncertainties of the percolation rates $\eta$ and the
Chapter 3. Uncertainty analysis

Figure 3.5: Marginals of the prior (dotted line) and posterior (solid line for the original model and dashed line for the improved model) distribution of the investigated hydrological soil parameters. Marginals of the prior are analytically calculated according to the distribution of the individual parameters listed in Table 3.1; Marginals of the posterior are estimated from the Markov sample, for the improved model this is the combination of multiple individual runs. The best parameter values of the optimization run for the improved model are indicated by a cross.
3.3. Results

E.: [math]
\begin{align*}
\text{percolation factors } f &= \text{dependent on the different soil types. Our prior assumption that the rates and factors for Cambisol and forest are somewhat higher than in Gleysols was confirmed.}

\text{The standard deviation of the error } \sigma &= \text{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.}
\end{align*}
\]
3.3.4 Uncertainties of spatial predictions

The spatially distributed model response was evaluated for the first major discharge event after herbicide application when the highest herbicide losses were observed (Leu et al., 2004a). Figure 3.7 shows the median and the 5 and 95% quantiles of the calculated surface runoff in the catchment during the main discharge event for the three simulations (prior prediction, prediction from calibrated original, and calibrated improved model). The prior prediction reveals very high uncertainty (Fig. 3.7a). In the 5% quantile, as well as for the median, only very few, mainly sealed areas, which are not relevant for herbicide losses, contribute to surface runoff. In contrast, in the 95% quantile most parts of the catchment produce surface runoff and are therefore prone to herbicide losses.

Using the calibrated original model, the prediction uncertainty was considerably lower when compared to the prior prediction (Fig. 3.7b). There are areas that contributed to surface runoff in all simulations and others that never contributed to surface runoff within the 95% confidence interval. Thereby, it must be mentioned that the calculated uncertainty bands for intrinsic model responses (e.g. surface runoff) only account for parameter uncertainties (see Discussion). In contrast, the uncertainty of the discharge prediction of the calibrated original and improved model reflects also structural and measurement error.

The effect of the improved model structure on the spatial uncertainty was much more pronounced. The calculated area of surface runoff (Fig. 3.7c) was smaller, because the percolation rates depending on the water table increased percolation during wet periods reducing the soil saturation in the topsoil. For example, if a perched water table of 50 cm is present, the new effective percolation rate is about 500 times higher. In this case, water flow is controlled by the hydrological conductivity in the bottom layer of the soil. The effect on the hydrology of the hydraulic gradient on drained areas that depend on the water table was smaller. Overall, the drain flow decreases through the lower water content in the soil.

In order to evaluate the spatial prediction of surface runoff on the agricultural fields we compared them with measured herbicide losses from the three subcatchments (Leu et al., 2004a). Thereby, we used the assumption that herbicides are mainly transported by fast flow processes and compared the amount of fast flow that is simulated (surface runoff that directly reaches the stream (="connected surface runoff ") and surface runoff that is connected by drain flow from sink areas) on the agricultural fields with the measured herbicide losses on these fields.
3.3. Results

Figure 3.7: 5, 50 and 95% quantiles of the simulated spatially distributed surface runoff in the study catchment on the 31st of May 2000 for a) the prior simulation, b) the calibrated original model and c) the calibrated improved model.

For all models (prior, calibrated original and improved model) the highest amounts of connected surface runoff are predicted for subcatchment 2 and very little fast flow reaching the stream is predicted for subcatchment 3. Both observations agrees well with the observed losses (Fig. 3.8). The predictions for subcatchment 1 are less successful. While the prior prediction showed an excellent agreement, both calibrated
models failed (at first sight) to simulate the relative differences to both other subcatchments. Interestingly, the model structure had a strong influence on the result. While the calibrated original model did hardly simulate any fast flow from subcatchment 1, the improved model predicted the highest amounts for this area. Based on field observations, the results from the improved model are much more realistic. Extensive generation of surface runoff during this rain event is confirmed by field observations showing large areas with ponding Frey et al. (see Fig. 3 in 2009). Hence, it seems that the improved model was successful in predicting the large amount of surface runoff in subcatchment 1 but probably overestimated the proportion of the ponded water that was quickly transmitted to the stream via preferential flow to tile drains.

Figure 3.8: Comparison of observed relative herbicide losses (left, Leu et al., 2004a) with the fast flow volume generated on the investigated corn fields during the rain event on the 31st of May 2000 actually reaching the stream in the three subcatchments predicted by three different models (prior simulation, maximum posterior density of the original and maximum posterior density of the improved model). The considered runoff processes are connected surface runoff (horizontally shaded) and preferential flow from sink areas (rest).
3.4 Discussion

3.4.1 Uncertainty of discharge prediction

Based on prior information only, the measured discharge values often laid outside the 90% bands of the prediction (Fig. 3.3). This indicated, since our prior are relatively wide, that parameter uncertainties are not the only relevant source of uncertainty and the incorporation of other error sources in an appropriated error model is essential. In the Bayesian inference approach, we incorporated an autoregressive error model that describes the effect of input, model structure, and measurement errors on the model output (stream discharge). The corresponding posterior uncertainty bands became wider, but much more realistic. However, careful analysis of the residuals and innovations (Fig. 3.4) clearly revealed systematic errors in the base flow calculation during dry periods that could not be accounted for by a modified error model. Through the conceptual modification of the original model, the simulation of the base flow dynamics could be significantly improved. Hence, the check of the inference assumptions regarding residual distribution and innovations was an important step to improve the quality of prediction. Additionally, this analysis indicated that the assumptions formulated in the likelihood function based on the improved model structure are in good agreement with the observed data.

The comparison between the original and improved model reveals the effect of model structure on the prediction uncertainty. The standard deviation of the error $\sigma$, and accordingly the uncertainty band, could be largely reduced due to the model improvement (Fig. 3.3 and Fig. 3.6). The reduction demonstrates that in the original model the structural deficits largely contribute to the prediction uncertainty. The remaining bias is due to other uncertainty sources. Depending on the situation, these can be uncertainty in measurements of the output response (e.g., discharge) or in input data (e.g., rainfall, evapotranspiration), as shown e.g. by Huard and Mailhot (2008).

3.4.2 Potential of discharge to constrain the parameter space

The range of certain parameters was significantly reduced by the additional information in the discharge data. A reduction was mainly observed for parameters which have large influence on the model result (sensitivity) and a large uncertainty in prior information (uncertainty). Examples are the measures of the pore-size distribution $N$ for different soils (sensitivity) and the percolation rates of Gleysol, Cambisol, and Calcareous...
Cambisol and the sink drainage efficiency parameter $M_{sink}$ (sensitivity and uncertainty). The calibration did not cause shifts of parameter values to regions of very low prior density. The limited extent of such shifts indicates that our prior knowledge was not in conflict with the information gained from the calibration data. A small shift towards higher values in the distribution could be observed for $\kappa$, the saturated hydrological conductivity $K_{sat}$ of different soils, and the percolation rate of Cambisol-Pseudogley. These parameters all increase the water flow in the soil and therefore accelerate the drying of the soil.

Spatially distributed parameters are hardly identifiable from data of a single watershed outlet alone. To overcome the problem of identifiability, we combined prior information of the model parameters with evidence from data using a Bayesian approach. In physically based models, at least some information is available for all parameters, either through literature data, other studies, or expert knowledge. There is no reason not to use such information for model predictions. In this way we can also calibrate a large number of parameters on a limited amount of information. However, sparse data limits the gain of information about the parameter values.

### 3.4.3 Spatial prediction of critical source areas

The identification of CSA has potential for mitigation of environmental impact while maintaining other positive externalities of agricultural production. However, the comparison of the spatial predictions yields some remarkable results. First, the spatial patterns differ substantially (Fig. 3.7) between the three models despite fairly similar discharge predictions (Fig. 3.3), similar observation were already made by Grayson et al. (1992). The improved model predicted much more restricted critical areas compared to both others and topography was clearly one of the main factors controlling the spatial extent of surface saturation. This result seems, based on field experience, much more plausible compared to the predictions of the two other models where surface saturation spread across nearly the entire catchment for the 95% quantile. Hence, improved model yields a much more sensitive relationship between the average degree of saturation of the soils and the discharge from the catchment. This agrees with the conceptual non-linearity that was introduced into the model by making the gradients for the percolation and drainage fluxes dependent on the water table.

The disadvantage of the applied error model is the fact that it only corrects the model output discharge, since it is only applicable for measured calibration data. Intrinsic model variables like surface runoff are not considered their estimated uncertainty is
based on parameter uncertainty only. Therefore, the spatial uncertainty ranges tend to be underestimated. This is a general disadvantage of correcting for deficiencies in model structure by an autoregressive error model to the output. A way to deal with uncertainty of intrinsic variables was developed by Reichert and Mieleitner (2009) who made model parameters time-dependent to account for structural deficits or sources of stochasticity directly where they occur.

The comparison between the fast flow prediction and the herbicide measurements also revealed the importance of model structure (Fig. 3.8). Due to the fact that all three models account for the effect of connectivity in the same way (Frey et al., 2009) they predict surface runoff mainly for subcatchment 2. The connectivity overrides the differences introduced by how the models represent water fluxes or how the models are calibrated. In contrast, the preferential flow from sink areas into the drainage system is directly driven by the calculated surface runoff on the sink areas and the sink drainage efficiency parameter $M_{sink}$. Based on the original model, there is little runoff and a smaller $M_{sink}$ in subcatchments 1 and 3. Hence, one would assume that there is little risk for herbicide losses. However, the herbicide measurements indicate considerable losses from subcatchment 1 which are well captured by the calibrated improved model. An absolute comparison between the two different fast flow processes in the three subcatchments and the measured herbicide losses is difficult because the concentration of the preferential flow through the drainage system and surface runoff is not equal. Based on field studies, concentrations in subsurface drains are usually much lower than in surface runoff (Kladivko et al., 2001). Overall, the evaluation reveals the importance of sink areas for herbicide losses, but also shows the uncertainty associated with the quantitative description of the process.

### 3.4.4 Convergence of Markov Chain

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 reached convergence or not. 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 we were restricted in the amount of possible simulations due to our computationally demanding simulation. With the original model structure, 34506 simulation runs could be carried out, with the modified structure two chains of 70702 and 58565 runs. We tested the convergence mainly by graphical analysis of the Markov chain.
For most parameters, it seems that the parameter space was adequately sampled by the Markov chains. Furthermore, the distribution also covered for most parameter the values of the optimization run in the range of the maxima. Only the linear baseflow coefficient (LBC) was not well covered. However, the comparison of the two Markov chains revealed that the sample size for some parameter was still too small and the accuracy is rather low.\(^2\) It is clearly a critical point in our analysis that, due to the computationally demanding simulations, our sample size is limited. An implication can be that not the entire parameter space was sampled and therefore the posterior uncertainty was underestimated.

It is a general problem that computationally demanding simulation models are restricted in their use for computer-intensive analysis techniques like Markov chains. However, more complex questions, such as the spatially distributed prediction of CSA, can often not be answered without such complex models. For this reason, efficient model implementation is crucial but, unfortunately, not the case for SMDR. Due to rewriting of parts of the code, the simulation time could be drastically increased. However, the program still needs 5 minutes for a 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 a restricted parameter space (O’Hagan, 2006). Emulators for dynamic models are still under development (Bhattacharya, 2007; Reichert et al., 2009). Parallel computing of multiple Markov chains would be another option (e.g. Vrugt et al., 2006).

### 3.4.5 Conclusions

When analyzing the extent of predicted CSA, the three models reveal important differences. Depending on the model structure, discharge data constrain the CSA extent to either a fairly large degree or hardly at all. Hence, the possibility to constrain the parameter space of a distributed model not only depends on the data to be used but also on the model. Discharge data are useful to reveal model structure deficits and also to calibrate and constrain parameters to which the calculated discharge is sensitive.

Despite the considerable differences in the saturated areas predicted by the three models, they all agree in predicting CSA at some locations and basically differ in the extent of the CSA around these “core” areas. This observation is primarily due to the fact that all three models assume saturation-induced runoff to be the mechanism of runoff formation. Accordingly, a large CSA predicted by one model should comprise a narrower

\(^2\)This will be improved for the version of this chapter which is currently under revision.
3.4. Discussion

CSA predicted by another model.

In the context of the field situation analyzed in this study, it seems that accounting for the connectivity between fields and stream is of major importance. For the ranking of the three subcatchments with respect to herbicide losses, connectivity overrides the differences between the models. Hence, a proper connectivity analysis based on a high-resolution DEM is a crucial, model-independent step that allows for a delineation of possible CSA (Frey et al., 2009).

It is necessary to further reduce the prediction uncertainty for agricultural risk areas. Discharge data are only an integrated catchment response. Spatial data could improve predictions a lot. For example it could be potentially useful to apply remote sensing data to map saturated areas (Troch et al., 2001) or to calibrate models by qualitative information like hydromorphological features from soil maps or multiple gauging stations.

Acknowledgements  We are indebted to Gérard S. Mohler and Daniele Passerone for their support with all the computer installation and to Pierre Gerard-Marchant and M. Todd Walter for introducing the SMDR model and Paul Sweeney and Irene Wittmer for ongoing stimulating discussions. Comments by Karim Abbaspour, Axel Bronstert, Tobias Doppler, Irene Hanke and Damian Helbling greatly improved the quality of the manuscript. The financial support of Syngenta Crop Protection is gratefully acknowledged.


Chapter 4

Comparison of different models to predict hydrologically sensitive areas for herbicide losses

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Abstract  Diffuse losses of agrochemicals from agricultural fields into surface waters generally originate from limited areas in a catchment. These areas are prone to fast flow processes and are also called hydrologically sensitive areas (HSA). Effective mitigation strategies to reduce these inputs rely on an accurate identification of these areas. We compared six approaches to identify HSA. We applied them to a small agricultural catchment in Switzerland, where spatial data on herbicide losses are available. The investigated approaches are a risk map integrated in the local soil map (FAL), an approach to delineate the Dominant Runoff Processes (DRP), an adaptation of the classification scheme of HOST (Hydrology Of Soil Types), a regression model to predict the spatial distribution of the Fast Flow Index (FFI), the topographic wetness index and the continuous physically-based water balance model SMDR (Soil Moisture Distribution and Routing). Despite their conceptual differences the spatial agreement in the prediction of risk classes is surprisingly high. The FAL risk map, DRP, HOST and FFI approaches are all based on the local soil map. In contrast, the topographic index and the SMDR are primarily based on the digital elevation model. This observation indicates that topography is reflected in the soil distribution in this landscape. If connectivity to the stream (on the surface and by the drainage system) is considered, the HSA predictions are in fair agreement with the observed spatial variability of herbicide losses.

Keywords: hydrologically sensitive areas (HSA); critical source areas (CSA); connectivity; herbicide losses; spatial modeling

4.1 Introduction

Agrochemicals are used to support crop growth by protecting them from pests or the competition with undesirable plants. Unfortunately, parts of the agrochemicals are transported away from their application site and may have negative side effects on non-target organisms. Therefore, it is a goal of environmental and agricultural policy to minimize adverse effects on the environment and human health (in Switzerland for example BAFU and BLW, 2008).

In this work, we focused on the risk of diffuse contamination of surface waters by agrochemicals, mainly herbicides. Diffuse losses from agricultural fields are in general limited to certain areas, also called hydrologically sensitive areas (HSA) (Walter et al., 2000). HSA are areas prone to fast flow processes, which are responsible for mobilization and transport of herbicides to the stream. A similar water quality concept is
4.1. Introduction

the delineation of critical source areas (CSA) (Pionke et al., 1996). The CSA definition additionally includes the availability of a substance (herbicides or phosphorus).

The HSA concept is substance independent since it focuses on runoff processes. HSA (respectively CSA) are strongly correlated with saturated areas since fast flow processes like surface runoff and macropore flow are mainly triggered by surface saturation in humid areas (Stamm et al., 2002). The slow transport through the soil matrix is less important since agrochemicals sorb and are degraded.

It has already been known for a longtime that limited parts of the catchment are prone to fast flow processes (partial area concept, Betson, 1964) and that the extent of those areas may vary with time (variable source areas concept, Hewlett and Hibbert, 1967). A reliable identification of HSA allows effective mitigation strategies like reduced application of agrochemicals or well placed buffer areas to reduce the contamination of surface waters by agrochemicals (Qiu, 2003).

Delineation of HSA has been investigated in various projects mainly focusing on phosphorus (e.g. Pionke et al., 2000; Heathwaite et al., 2005). Different approaches exist to identify such areas, from simple indices to more complex, physically based models. Different simple hydrological approaches to delineate HSA are for example explored by Srinivasan and McDowell (2007). An analysis of the predictive power of terrain indices for saturated areas is given by Günther et al. (2004). Examples of more sophisticated physically based modeling approaches to simulate spatial variability are the models SMD/SMDR (e.g. Frankenberger et al., 1999; Gerard-Marchant et al., 2006; Frey et al., 2009) or TOPMODEL (e.g. Quinn and Beven, 1993). Despite promising results, spatial predictions still involve large uncertainties, especially about the model structure. Furthermore, spatially distributed validation data are often lacking.

In this work, we investigated the spatial HSA prediction of six approaches in a small agricultural catchment. Previous intensive field investigations revealed large spatial heterogeneity of herbicide losses among three subcatchments (e.g. Leu et al., 2004a,b; Gomides Freitas et al., 2008). These measurements of the spatial variability of herbicide losses allow us to partly test the different approaches.

The first approach is the risk classification integrated in the local soil map (FAL and Kanton Zürich, 1996). It classifies the susceptibility of agricultural land to transport processes based on pedological information interpreted by expert judgment. Secondly, we applied the Dominant Runoff Processes (DRP) approach (Scherrer and Naef, 2003; Schmocker-Fackel et al., 2007). It aims at predicting the dominant runoff process in the landscape. In a similar way, the Hydrology Of Soil Types (HOST) developed in the
Chapter 4. Model comparison

United Kingdom (Boorman et al., 1995) classifies the dominant flow paths and links the HOST classes to the Base Flow Index (BFI), derived from a multiple linear regression. The BFI corresponds to the long-term average proportion of the discharge that occurs as base flow. Empirical data suggest a close link between the BFI or the Fast Flow Index (FFI=1-BFI) and the vulnerability of a catchment for herbicide losses (Leu et al., in prep.). This is the rational of the fourth approach which consists of predicting the FFI based on soil and topographic attributes according to a multiple regression analysis (Siber et al., 2009). The fifth approach is the topographic (wetness) index (\(\lambda\)) (Beven and Kirkby, 1979). Studies of Güntner et al. (2004) and Agnew et al. (2006) revealed that this is, in a comparison with other indices, the most appropriate index to identify saturated, respectively hydrologically sensitive areas. Finally, we included the continuous physically-based water balance Soil Moisture Distribution and Routing model (SMDR) in our comparison. Its objective is to predict the spatial pattern of critical source areas (Frankenberger et al., 1999; Soil and Water Laboratory, 2003; Gerard-Marchant et al., 2006). We had applied this model to our study catchment in earlier investigation and had adapted it to the local conditions by incorporating artificial drains, surface connectivity and a water table dependent percolation (Frey et al., 2009, submitted).

The objective of this work was to compare the conceptually different approaches and evaluate them with spatially distributed herbicide losses. Furthermore, we analyzed their differences, advantages and limitations with regards to practical applications. An approach should be straightforward to apply and be based on easily available data. However, a critical point for the practical application is the reliability of the prediction. In the Methods section, we introduce the study area and the available information, the theoretical background of the applied approaches and their practical application. In the Result section the different predictions are compared and validated against field measurements. The discussion part at the end closes with environmental implications including suggestions for practical management options.

4.2 Methods

4.2.1 Study area and validation data

Our studied catchment is a small agricultural watershed of 1.9 km\(^2\) within the Swiss Plateau. It is characterized by moderate slopes. Its geologic underground is formed out of molasse from tertiary river deposits, moraines and drumlins. The catchment can be divided in three subcatchments (aerial picture in Fig. 4.1).
4.2. Methods

The herbicide loss dynamic in the catchment was intensively analyzed during the growing seasons 1999 (Leu et al., 2005), 2000 (Leu et al., 2004a,b) and 2003 (Gomides Freitas et al., 2008). The most comprehensive study took place in 2000. In a controlled herbicide application, a defined herbicide mixture (including atrazine, dimethenamid and metolachlor) was applied to all corn fields in the catchment. All applications were carried out on the same day, thus the herbicides on all fields were exposed to the same weather conditions. The applied herbicides were not used on any other field in the catchment during that growing season.

In the weeks following the application, discharge and herbicide concentrations were monitored in the streams at the outlets of the three subcatchments (labeled 1, 2, and 3 in Fig. 4.1). The main herbicide losses occurred during the first rain-discharge event after the application, mainly by fast flow processes like surface runoff and macropore flow to the drainage system. A large spatial variability of the herbicide losses between the subcatchments was observed. The losses in subcatchment 2 were over 50 times larger than those in subcatchment 3, the losses in subcatchment 1 were in-between (Leu et al., 2004b).
4.2.2 Data

Predictions of HSA rely on spatially distributed input information. Available data are a digital elevation model (DEM) with 2 m resolution (DTM©2003 swisstopo, JA082266) upscaled to a resolution of 25 m, a soil map (1:5,000) (FAL and Kanton Zürich, 1996), land-use data with 25 m resolution (Flury et al., 2004), a geological map (Bundesamt für Landestopografie swisstopo, 2007), a map with subsidized drains (AWEL, 1990), and a map with the surface connectivity derived from the 2 m resolution DEM (Frey et al., 2009) (Fig. 4.2).

The risk approaches were calculated with a resolution of 25 m. Settlements and woods are neglected in the FAL risk map, DRP and HOST approaches.

4.2.3 HSA prediction tools

In the first subsection we summarized the main conceptual features of all six approaches. The technical details are described in 4.2.3 for each method.

Theoretical background

The FAL risk map is part of the soil map 1:5,000 (FAL and Kanton Zürich, 1996). It qualitatively classifies the susceptibility of agricultural areas to lose nutrients and is for example used for manure application recommendations. Since transport processes for phosphorus are similar to those of mobile pesticides, it can also be applied for predicting HSA. Four risk classes are distinguished ranging from a low risk (class 1) to a very high risk (class 4). Additionally, the factor that mainly controls the risk classification is indicated.

A decision tree to assess the Dominant Runoff Processes (DRP) was introduced by Scherrer and Naef (2003). Schmocker-Fackel et al. (2007) simplified and generalized the decision tree to delineate DRP automatically on the basis of soil, topography and geology for entire catchments in the Swiss Plateau. This method distinguishes between Hortonian overland flow (HOF), saturated overland flow (SOF), natural subsurface storm flow (SSF), artificial drain flow (D), and deep percolation (DP). Additionally, three storage capacity categories 1, 2 and 3 are attributed to the runoff processes HOF, SOF, SSF and D. The number indicates how sensitively an area reacts to rainfall. A higher number indicates a more delayed runoff formation. Relevant transport processes for herbicide transport are overland flow, drain flow and to a lesser extent
4.2. Methods

Figure 4.2: Available spatially distributed data in the study catchment: a) elevation, b) soil map, c) land use, d) geology, e) areas with subsidized drains and f) surface connectivity. Boundaries of the corn fields of the field study 2000 and the stream (dotted line where it flows in a culvert) are delineated.
subsurface storm flow. Areas with deep percolation are no HSA for surface waters.

The Hydrology Of Soil Types (HOST) approach was established to allow a direct use of available information on soils and their distribution for hydrological purposes (Boorman et al., 1995). The approach developed for soils in the United Kingdom was used for low flow and flood estimations in ungauged catchments. Schneider et al. (2007) successfully adapted the HOST approach to the major parts of Europe based on the soil geographical database of Europe. Based on the associated BFI, respectively FFI, the HOST approach can be used to predict risk areas for water quality. Herbicide pollution is mainly triggered by fast flow processes and therefore linked with the FFI (Leu et al., in prep.); the higher the FFI of a soil the higher its risk for herbicide losses.

The same idea is also used in the approach of Siber et al. (2009). They calculated a regression function for the FFI based on 57 investigated catchments in the Swiss Plateau. The FFI, calculated from the catchment discharge, was related to spatial attributes of the catchment: topographic, climatologic, land use and soil data were used. The investigation also included a regression analysis of a subset of 22 catchments in the Canton of Zurich. For this regression a soil map with a finer resolution was available. Since our catchment is within the Canton of Zurich we focused on this regression.

The topographic index $\lambda$ is based on the assumption that topography, respectively gravity is the driving force of water movement. $\lambda$ combines the upslope contributing area with the local slope to describe the spatial distribution of soil moisture. The upslope area is a proxy for the amount of water inflow from upslope and the slope describes how fast the water is transferred downslope. Areas with a high tendency of surface saturation are strongly linked with risk areas for herbicide pollution, since the relevant fast flow processes are primarily triggered on saturated areas.

The Soil Moisture Distribution and Routing model (SMDR) is a physically-based distributed water balance model that allows for calculating the spatial extent of saturated areas and runoff generation. In contrast to the other approaches, SMDR is continuous in time and can calculate the temporal variability of HSA.

Beside the temporal variability, connectivity is a further critical point for the delineation of HSA. Not all areas are directly connected to the stream. Connectivity describes the direct connection of an area with the river system through fast flow pathways. This can either be on the surface (surface runoff) or through preferential flow paths (macropore flow from sink areas into the drainage system). To assess the surface connectivity and sink areas we use a map which is calculated based on a high resolution digital elevation map (Fig. 4.2f). Their derivation is described in Frey et al. (2009). The extent of the drainage system is assessed by a drainage map (Fig. 4.2e).
4.2. Methods

Technical details

FAL risk map

A general decision scheme to obtain the risk rating is shown in Fig. 4.3. It is based on data provided by the soil map. The main soil attributes used for the classification are the water regime class, soil depth, texture and slope. It is assumed that transport processes either occur through overland flow to a surface water body or through leaching to the groundwater. The risk factors for overland flow are large slope, poor drainage, small storage capacity and a high groundwater table or large lateral water inflow. A highly permeable underground is assumed to increase the risk for leaching. The risk class gets higher as the water logging increases, the storage capacity decreases, the grain size is unfavorable and the slope is steeper.

The final classification is determined by the limiting factor that causes the maximum risk. If the maximum risk classes of the slope and of another factor are equal, slope predominates. More details about the deviation of the risk map are given in FAL and Kanton Zürich (1998).

Classification of Dominant Runoff Processes

The decision scheme to generate the DRP map on agricultural land is depicted in Fig. 4.4. First, it is decided whether Hortonian overland flow has to be expected. If the surface is artificially sealed, HOF 1 occurs. Otherwise, it is assessed whether the area is susceptible to soil surface sealing or compaction and therefore to a limited infiltration capacity resulting in HOF 2. Since it is assumed that Hortonian overland flow only occurs during intensive rainfall, these soil units are additionally classified with respect to SOF, SSF, D and DP for less intensive but longer rainfall events.

The dominant runoff process on highly permeable soils without groundwater influence is DP. Otherwise, the dominant runoff process of a soil unit is either classified as D on drained areas, SSF if the slope exceeds 15 % or SOF. The storage categories of the processes correspond to the storage capacity of the soil. The storage capacity is calculated as the product of the depth to the vertical percolation barrier (impermeable layer and/or water logging) times the drainable porosity (porosity between field capacity and saturation). Storage class 1 ranges from 0 to 40 mm, storage class 2 from 40 to 100 mm and storage class 3 from 100 to 200 mm. Storage capacities exceeding 200 mm are classified as DP.
Chapter 4. Model comparison

Figure 4.3: Decision scheme to assess the risk classes (according to FAL and Kanton Zürich, 1998).

HOST

Based on available information from the soil and the geology map interpreted by a local expert we derived a decision tree to classify the soils in the study catchment according to the HOST classification (Fig. 4.5). First, the geology types were assigned to the substrate hydrogeology categories defined in Boorman et al. (1995). Molasse and moraine material were considered as slowly permeable substrate, drumlins to unconsolidated soils and unclassified area (mainly wet areas) to raw peat soil. Secondly, the depth of an impermeable or gleyed layer was derived from the soil water regime classes used in the soil map (Table 4.1).

Finally, the distinction between HOST class 18 and 21 was made based on the integrated air capacity (IAC). This is the volume of pores with a diameter exceeding $60 \, \mu m$. Those pores are assumed to be unable to retain water against gravity. The pressure head to drain such pores corresponds roughly to 0.5 m of water. IAC is calculated from the difference between the water content at saturation and the water content at 0.5 m pressure head. The water content, $\theta$, at a certain pressure head, $h$, was calculated
4.2. Methods

Figure 4.4: Decision scheme to determine the dominant runoff processes (according to Schmocker-Fackel et al., 2007).

Table 4.1: Relationship between the soil water regime in the local soil map and the vertical distance to an impermeable or a gleyed layer.

<table>
<thead>
<tr>
<th>soil water regime class</th>
<th>impermeable and/or gleyed layer</th>
</tr>
</thead>
<tbody>
<tr>
<td>well-drained soils</td>
<td>no impermeable or gleyed layer within 100 cm</td>
</tr>
<tr>
<td>influenced by groundwater or stagnant water in the profile</td>
<td>impermeable layer within 100 cm or gleyed layer at 40-100 cm</td>
</tr>
<tr>
<td>dominated by groundwater or stagnant water in the profile</td>
<td>gleyed layer within 40 cm</td>
</tr>
</tbody>
</table>
Figure 4.5: Decision tree to classify the subsoil in the catchment into the HOST scheme.

according to the equation of van Genuchten (1980):

\[
\frac{\theta - \theta_r}{\theta_{sat} - \theta_r} = \frac{1}{(1+|\alpha h|)^M}
\]

\[
\text{with } M = 1 - \frac{1}{N}
\]

thereby \( \theta_r \) is the residual water content, \( \theta_{sat} \) the water content at saturation, \( \alpha \) the inverse air entry suction, and \( N \) a measure of the pore-size distribution. These parameters are not directly available in the soil map. We derived them using pedotransfer functions of the Rosetta software (Schaap et al., 2001). Texture data from soil profiles in the soil map were used as input (details in Frey et al., 2009).
4.2. Methods

The classified HOST classes in the catchment are associated with a base flow index (BFI) according to the calculations of Boorman et al. (1995) (Table 4.2). Where available the BFI derived in the work of Schneider et al. (2007) for Europe are added to the table for comparison. The FFI, which is relevant for the delineation of HSA, can be directly derived from the BFI:

\[
FFI = 1 - BFI
\]  
(4.2)

Table 4.2: Base flow index and fast flow index for the HOST classes in the study catchment (Boorman et al., 1995; Schneider et al., 2007).

<table>
<thead>
<tr>
<th>HOST class</th>
<th>Boorman et al. (1995)</th>
<th>Schneider et al. (2007)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>BFI</td>
<td>FFI</td>
</tr>
<tr>
<td>5</td>
<td>0.90</td>
<td>0.10</td>
</tr>
<tr>
<td>13</td>
<td>1.00</td>
<td>0.00</td>
</tr>
<tr>
<td>14</td>
<td>0.38</td>
<td>0.62</td>
</tr>
<tr>
<td>16</td>
<td>0.78</td>
<td>0.22</td>
</tr>
<tr>
<td>18</td>
<td>0.52</td>
<td>0.48</td>
</tr>
<tr>
<td>21</td>
<td>0.34</td>
<td>0.66</td>
</tr>
<tr>
<td>24</td>
<td>0.31</td>
<td>0.69</td>
</tr>
<tr>
<td>29</td>
<td>0.23</td>
<td>0.77</td>
</tr>
</tbody>
</table>

Fast Flow Index (FFI) approach

In the multiple regression analysis the influence of catchment attributes (including topographic, climatic, land use and soil data) on the FFI (calculated from measured discharge data) of the investigated catchments resulted in the following relationship:

\[
FFI = -0.615 + 0.131 \cdot \rho_{river} + 0.013 \cdot f_{soil}
\]  
(4.3)

where \(\rho_{river}\) is the river density and \(f_{soil}\) is a numerical factor which describes the soil water regime from well drained (numeric value 1) to permanently saturated (numeric value 8) soils (Table 4.3).
Table 4.3: Classification of the soil water regime classes from the soil map into the regression classes

<table>
<thead>
<tr>
<th>soil water regime class</th>
<th>regression class: $f_{soil}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>permeable, well-drained</td>
<td>1</td>
</tr>
<tr>
<td>forest</td>
<td>1</td>
</tr>
<tr>
<td>well-drained with some influence of groundwater</td>
<td>2</td>
</tr>
<tr>
<td>stagnant water, rarely saturated to the surface</td>
<td>3</td>
</tr>
<tr>
<td>stagnant water, often saturated to the surface</td>
<td>4</td>
</tr>
<tr>
<td>influenced by groundwater, rarely saturated to the surface</td>
<td>5</td>
</tr>
<tr>
<td>influenced by groundwater, often saturated to the surface</td>
<td>6</td>
</tr>
<tr>
<td>influenced by groundwater, most of the time saturated to the surface</td>
<td>7</td>
</tr>
<tr>
<td>influenced by groundwater, always saturated to the surface</td>
<td>8</td>
</tr>
<tr>
<td>urban areas</td>
<td>8</td>
</tr>
</tbody>
</table>

**Topographic (wetness) index ($\lambda$)**

The topographic index, $\lambda [\ln(T)]$, was calculated with the following equation:

$$\lambda = \ln \left( \frac{\alpha}{\tan(\beta)KsD} \right) \tag{4.4}$$

where $\alpha$ is the upslope contributing area, $\beta$ the local slope, $K_s$ the saturated hydraulic conductivity and $D$ the soil depth. The ratio $\alpha/\tan(\beta)$ was calculated with the software package TOPMODEL of R (http://cran.r-project.org). The product of $K_s$ and $D$ stands for the soil transmissivity. Their spatial distribution was taken from the soil map (FAL and Kanton Zürich, 1996). The same values as in Frey et al. (2009) were used.

**Soil Moisture Distribution and Routing model**

In the SMDR the catchment area is divided into a uniform grid. Each grid unit consists of multiple homogeneous horizontal layers of varying thickness which divide the units into cells. The considered exchange processes between the different cells are displayed
in Fig. 4.6. The model runs on a daily time step and calculates the water balance of each cell for every time step. River flow is not explicitly considered and discharge is calculated only at the outlet of the catchment.

The model is driven by rain input into the top layer. The water flow in lateral and vertical direction is calculated based on Darcy's law. To account for preferential flow the hydraulic conductivity above a certain water content is multiplied with a factor which exponentially decreases with depth. The lateral water distribution to cells downhill is based on the algorithm of Tarboton (1997). In the modified version we assumed that the lateral flow is intercepted by subsurface drains if present; the flow is therefore directly routed to the river (catchment outlet) (Frey et al., 2009). The lateral hydraulic gradient on drained areas is a function of the water content of the entire profile (Frey et al., submitted). In the remaining catchment, the hydraulic gradient relevant for lateral flow is assumed to be equal to the local slope. At the bottom of the soil profile deep percolation to a linear base flow reservoir takes place. The percolation rate is a linear function of the water table in the soil profile (Frey et al., submitted). At the soil surface, outflow through evapotranspiration is considered. At the end of the daily time step all water in excess to the water storage capacity of a layer is routed to the overlying layer. At the soil surface, excess water is converted into overland flow, which is directly routed to the catchment outlet. However, since large parts of the catchment are not directly connected to the river in our catchment we account for the re-infiltration of
surface runoff in sink areas where water can accumulate (Frey et al., 2009). If such a sink area is artificially drained, a secondary drainage component was introduced that comprises possible macropore flow to tile drains.

SMDR requires spatially distributed information about the hydrological properties, land use, elevation and some general data (e.g. drainage coefficient). The parameterisation steps are explained in Frey et al. (2009). For the comparison in this article we used parameter values derived from a Bayesian parameter estimation calibrated with discharge data (described in Frey et al., submitted).

The simulation with SMDR results in continuous time series of spatial data with a daily time step. For a general risk assessment, we carried out a long-term simulation over 10 years (1998 to 2007) and calculated the average top soil saturation and average surface runoff over this period. The winter months (November to March) with possible snow accumulation were excluded from the calculation. The average annual precipitation accounted for 1310 mm, ranging from 1040 to 1670 mm.

### 4.2.4 Definition of comparable risk classes

To compare the different models we classified the output of all approaches into three risk categories (1: high risk, 2: medium risk, 3: low risk) (Table 4.4). Since we focused on HSA for surface waters, risk for groundwater contamination was excluded. For the FAL risk map the three risk categories high, medium and low risk were adopted directly. In our catchment the category very high risk is always associated with the risk factor permeable underground, which indicates risk for groundwater contamination. Therefore, we reclassified it as low risk for surface waters. In the DRP approach, areas with a high sensitivity to rainfall (D1, SOF1, SSF1) were put into the high risk category. D2, SOF2, SSF2 were considered as medium and D3, SOF3, SSF3, DP as low risk. The distribution of both approaches shows about 20% high, 30% medium and 50% low or not classified risk areas (see below Fig. 4.8 in section 4.3.2). The bounds of the classes of the remaining approaches were chosen in a way that the resulting distributions of the risk classes were similar. The connectivity was ignored for the delineation of the risk areas.
Table 4.4: Comparable risk classes

<table>
<thead>
<tr>
<th>approach</th>
<th>original risk classes</th>
<th>comparable risk class for surface water</th>
</tr>
</thead>
<tbody>
<tr>
<td>FAL risk class</td>
<td>high risk</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>medium risk</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>low risk</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>very high risk associated with risk for groundwater percolation</td>
<td>3</td>
</tr>
<tr>
<td>DRP</td>
<td>D1, SOF1, SSF1</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>D2, SOF2, SSF2</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>D3, SOF3, SSF3, DP</td>
<td>3</td>
</tr>
<tr>
<td>HOST</td>
<td>class 29</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>class 24</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>classes 5, 13, 14, 16, 18 and 21</td>
<td>3</td>
</tr>
<tr>
<td>FFI</td>
<td>FFI &gt; 0.7</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>0.7 ≥ FFI &gt; 0.4</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>FFI ≤ 0.4</td>
<td>3</td>
</tr>
<tr>
<td>λ</td>
<td>λ &gt; 9.87</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>9.87 ≥ λ &gt; 7.72</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>λ ≤ 7.72</td>
<td>3</td>
</tr>
<tr>
<td>SMDR</td>
<td>runoff &gt; 2 %</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>average saturation &gt; 42% and runoff ≤ 2%</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>average saturation ≤ 42% and runoff ≤ 2%</td>
<td>3</td>
</tr>
</tbody>
</table>

4.3 Results

4.3.1 Model predictions

The FAL risk classes derived from the soil map predict HSA for large parts of the flatter areas along the river where the agricultural fields are situated (Fig. 4.7a). The risk factor for these areas is a high groundwater table.

Towards the hillslopes, medium risk (risk factor: high groundwater table, small storage capacity or poor drainage) or even low risk is predicted. Very high risk is only predicted in combination with the risk factor permeable underground and therefore indicating a
Figure 4.7: Prediction of risk areas in the study catchment based on different approaches: a) FAL risk map; b) DRP; c) classification after HOST; d) FFI based on a regression model; e) topographic index; f) average surface saturation over 10 years (without winter months) calculated with SMDR; g) average surface runoff events over 10 years (without winter months) calculated with SMDR, connected surface runoff is shaded. Boundaries of the corn fields of the field study 2000 and the stream (dotted line where it flows in a culvert) are delineated.

The DRP approach predicts a high potential for drainage flow for the agricultural fields in subcatchment 1 (Fig. 4.7b). A high potential for saturated overland flow has to be expected for areas situated along the river. On the investigated corn fields high risk for overland flow is predicted in subcatchment 2. For the agricultural fields in subcatchment 3 medium risk for drainage flow and surface runoff is predicted. Subsurface storm flow or deep percolation is predicted only for smaller areas at the border of the catchment without intensive agriculture.

The risk of the different HOST classes (Fig. 4.7c) can be assessed by analyzing the predicted fast flow indices (Table 4.2). The highest amount of fast flow is predicted for HOST class 29 (77% of the total discharge), which is located in the flat areas of the catchment. The second highest risk for fast flow is predicted for HOST class 24.
(69%), followed by class 21 (66%). These classes are spatially situated around class 29. These three classes cover most of the investigated agricultural fields. Only two fields (one in subcatchment 2, one in 3) are in HOST class 16, which has a clearly lower FFI (22%).

The FFI approach yields a continuous risk scale instead of categories (Fig. 4.7d). The highest FFI is predicted for the flat area in subcatchment 1. According to the regression equation the FFI increases towards the stream. Furthermore, it increases towards the catchment outlet because of the increasing river density.

The topographic index $\lambda$ varies between 4.5 [ln(T)] on the ridges to 19.5 in the flat subcatchment 1 (Fig. 4.7e). In contrast to the previous approaches the topographic index has a higher small-scale variability. This is caused by the fact that the underlying DEM with a 25 m resolution has much more variation then the soil data which dominate in the other approaches.

From the SMDR simulation the average saturation over ten years is shown in Figure 4.7f. Spots with higher water contents are located in the flat area in subcatchment 1 and around the streams in the entire catchment. Agricultural fields in all three subcatchments are partially exposed to high saturation. The SMDR results in a high small-scale variability similar to the topographic index. SMDR also predicts surface runoff (Fig. 4.7g). The surface runoff pattern follows closely areas with high saturation. Based on surface runoff the importance of surface connectivity can be demonstrated. Only from shaded areas in Figure 4.7g surface runoff directly reaches the stream. Due to topographic barriers some surface runoff is retained in sink areas (Frey et al., 2009). However, if sink areas are drained, runoff can reach surface waters via preferential flow paths (macropores and drains).

### 4.3.2 Spatial model comparison

The different approaches were compared by calculating the difference of the spatially predicted risk classes (Fig. 4.8). Diagonally the risk classes derived from the different models are given. According to our intent, the distribution of the risk classes of the different approaches is comparable. High risk areas cover from 12% (HOST) to 25% of the area (FAL risk map), medium class from 27% (SMDR) to 32% (DRP) and low risk from 37% (FAL risk map and DRP) to 52% (SMDR). The maximum fraction of unclassified area is 9% (FAL risk map, HOST, and DRP).

The agreement between the different approaches is fairly good. The comparison shows that for most parts of the catchment the risk classes are identical (from 47% up to 75%
Figure 4.8: Spatial comparison of the different approaches: Diagonally the risk classes derived from the different approaches are given. 1 indicates a high risk, 2 a medium and 3 low, non-classified areas are called NA. These maps are then subtracted from each other. A negative value indicates that the risk in the first mentioned approach is higher, a positive value that the risk in the latter is higher, at 0 both maps are equal. These maps are given in the upper right part of the plot. In the lower left part a histogram with the distribution of the deviation is shown.
of the area). Large deviations by 2 classes are rare (maximum 9%). The best match exists between the FAL risk map and the DRP approach. The physically based SMDR and the $\lambda$ approaches differ more from the other approaches and from each other as well.

To combine the different approaches, we calculated the average, the maximum, and the minimum risk, as well as the average deviations of all predictions (Fig. 4.9). Parts of the flat area in subcatchment 2 are identified as high risk areas in all approaches. Other parts of the catchment are more controversial, for example the ridges in the east of the catchment, where the average deviation is higher. Most approaches predict a low risk; however, with the FAL risk map a high risk is predicted.

![Figure 4.9: Average (a), lower (b) and upper (c) boundaries and average deviation (d) for the risk classes of all the analyzed models (risk map, DRP, HOST, FFI, $\lambda$ and SMDR).](image)

### 4.3.3 Validation with measured herbicide losses

The predicted risk classes for the investigated fields based on the different models can be compared with measured herbicide losses from the 3 subcatchments to test the different approaches (Fig. 4.10).

The field study revealed that the herbicide losses from fields in subcatchment 2 were clearly higher than in subcatchment 1 and much higher than in subcatchment 3 (Fig. 4.10a). Without considering surface connectivity and drains, the measured difference between subcatchment 1 and 2 could not be reproduced by any risk model. In all approaches there are clearly less high risk areas in subcatchment 2 than in subcatchment 1. In subcatchment 3 only few high risk areas are predicted, which is in agreement with the low measured herbicide losses. The exception is the FAL risk map approach, which largely overestimates the high risk areas in subcatchment 3.

It is crucial to take the connectivity into account to explain the spatial distribution of the
Figure 4.10: Comparison between measured herbicide losses during the field study of Leu et al. (2004a) a) and distributions of predicted risk classes on the investigated agricultural fields in the different subcatchments for the different approaches b)-g). Thereby only on the diagonally shaded proportion of the areas surface runoff is connected to the river, whereas the perpendicular shaded areas are drained.
herbicide losses. There are no surface connected agricultural fields in subcatchment 1, whereas large parts of the fields in subcatchment 2 are directly connected to the stream. The few surface connected areas in subcatchment 3 correspond in general to medium and low risk areas. Instead, large parts of the predicted high risk areas in subcatchment 1 are drained, whereas there are no drains in subcatchment 2. In subcatchment 3 only the FAL risk map approach shows drained high risk areas.

4.4 Discussion

4.4.1 Connectivity

The investigated approaches assess the local vulnerability to produce fast flow and do not account for any kind of connectivity (exception SMDR, see below). Only by including the surface connectivity (Fig. 4.2f) and the drainage system (Fig. 4.2e) into our considerations the observed herbicide losses can be understood. According to our knowledge, surface runoff on HSA is responsible for the mobilization of herbicides on agricultural fields. If the field is surface connected to the river system, herbicides are directly transported to the surface water (e.g. subcatchment 2). However, due to topographic barriers, surface runoff can not directly reach the river system in large parts of the catchment. On those unconnected areas, surface runoff will re-infilt rate in sink areas. If the sink areas are nearly saturated, macropore flow is initiated. On drained areas, macropore flow can be connected directly to the drainage system, which is further connected to the river system. Thus, herbicides will still reach the stream (e.g. subcatchment 1). However, due to sorption and degradation the losses through drains are smaller compared to direct surface runoff. Kladivko et al. (2001) concluded from over 30 studies that pesticide concentrations and mass losses through subsurface drains are usually much lower compared to surface runoff, often by an order of magnitude. This explains why the observed herbicide losses from subcatchment 1 are lower than from subcatchment 2 despite the high percentage of high risk areas.

The high risk for fast flow in subcatchment 1 could be attested in multiple field inspections. During and shortly after large rain events, we observed extensive surface runoff on the agricultural fields. Due to topographic barriers, in this case a slightly raised field road, surface runoff is stopped from running into the stream and large ponding areas were observed (Fig. 4.11).

A concept about connectivity is given by Ambroise (2004). He proposed, in extension
to the variable source area concept, that an area has to be hydrologically active and connected to the catchment outlet to become a “contributing” area. Another study that supports our finding is the one of Richards and Brenner (2004). They also revealed that a large part of their catchment did not directly contribute to catchment outflow. Furthermore, they observed that anthropogenic features like drains can increase the area contributing to the catchment outlet. However, the influence of surface connectivity on solute transport is often neglected. Richards and Brenner (2004) supposed that the main reason for overlooking the surface connectivity is the fact that sinks in DEM are interpreted as errors in general terrain analysis.

As shown here, the incorporation of connectivity in a risk approach is not difficult. An existing risk approach can be overlaid with surface connectivity and drainage information. Surface connectivity and sink maps can be derived from a DEM. Thereby, a high-resolution DEM is necessary since small scale structures can be crucial (Frey et al., 2009). Such high-resolution DEM based on Airborne-Laser-Scanning are becoming more and more available. Complete drainage maps are often difficult to obtain, but are occasionally available. A possible new way to produce drainage maps is their delineation based on aerial pictures (Tetzlaff et al., 2008).

In the modified version of SMDR, surface connectivity is already considered (Frey et al., 2009). However, for the determination of the risk classes connectivity was not taken into account. In the simulation surface connectivity and re-infiltration of surface runoff in sink areas was calculated. Therefore, due to the water re-infiltration the simulated surface saturation for sink areas was actually slightly higher than without connectivity. The
application of the modified SMDR approach has some disadvantages. SMDR is by far the most time and data consuming approach and its application with fine resolution on a larger scale demands great computer resources. Since the surface connectivity map is produced outside of SMDR, it is also a promising option to couple surface connectivity with other approaches.

4.4.2 Differences between the approaches

The investigated approaches can help to further differentiate the risk for herbicide losses of agricultural areas and improve the effectiveness of management actions. Despite their conceptual difference, the spatial agreement in the prediction of risk classes of the investigated approaches is relatively high. Certain areas in the flat area in subcatchment 1 for example are classified as high risk by all approaches (Fig. 4.9). FAL risk map, DRP, HOST, and FFI approach have the highest agreement. This can be explained by the fact that they are all primarily based on the soil map. In contrast, the topographic index $\lambda$ is primarily based on the digital elevation model and SMDR incorporates both data. The approaches based on the DEM result in a higher spatial variability than the approaches based on the soil data because the DEM has a higher spatial variability whereas the resolution of the soil map is coarser. The core of the high risk areas is similar in all approaches.

The similarity of the predictions in all approaches indicates the correlation between topography and soil. The soil classes also reflect some topographical aspects of a catchment because topography is an important factor for the pedogenesis (Jenny, 1994).

Our calculation of $\lambda$ incorporated the transmissivity and therefore also soil specific information. However, $\lambda$ can also be applied without transmissivity. A spatial comparison showed that $\lambda$ predictions with and without transmissivity are very similar. 85% of the risk classes are equal and the maximum deviation was only one class (data not shown). Thus, the influence of the transmissivity is small in this case and $\lambda$ could also be applied without soil data.

Our results suggest that the surface topography is a strong predictor for the surface saturation and the water transport. However, the water flow is probably more dominated by the bedrock than the surface topography (e.g. Freer et al., 2002). Unfortunately, bedrock topography is much more difficult to determine than the surface topography. Furthermore, in less topographically dominated landscapes topography has less influence on the water flow and other factors gain importance (e.g. hydrological soil properties).
Chapter 4. Model comparison

The FAL approach predicts an unrealistic high risk on the agricultural fields in subcatchment 3 (Fig. 4.10b). A soil profile in the Gleysol in subcatchment 3, analyzed during the field study, exposed a sandy soil in the underground layer which is not included in the soil map. This leads to an overestimation of the risk class in the soil map. In the DRP, HOST, and FFI the missing layer has less influence. In SMDR and $\lambda$ the sandy layer was explicitly integrated (Frey et al., 2009).

It is a weakness of the FAL approach that it does not consider interactions between the risk factors. This is demonstrated by another deviation of the FAL risk map compared to the other approaches. In the east of the catchment the risk map exhibits a high risk. The risk factor “small storage capacity” is caused by the thin soil layer. However, through the large hydrologic gradient the storage is also drained very efficiently which reduces the risk.

4.4.3 Temporal variation of HSA

A universal determination of risk areas is not possible, since, in accordance to the variable source area concept, the spatial extent of HSA depends on the rain event and the preconditions. However, as described in the Methods section, most of the investigated approaches are static. Gburek et al. (2000) used the return period concept to include the temporal variation into the static phosphorus index approach. The return period describes the probability of a rainfall of a given magnitude. They developed a relationship between the peak flow and the contributing area adjacent to the stream. This concept would also be applicable together with our investigated approaches.

Schmocker-Fackel et al. (2007) also used the DRP approach to quantify storm runoff. Thereby, storage capacities of 20 mm, 70 mm, and 150 mm were attributed to the storage classes 1 to 3. To account for the preconditions the storages were filled with the 5 day pre-event rainfall during summer (May - September) and the 10 day pre-event rainfall during winter (October - April). Depending on the size of the rain event different storage classes are filled and the extent of HSA expands. However, large jumps in the extent of HSA occur due to the coarse discretisation in only three classes.

SMDR allows for considering the temporal variation explicitly. Instead of averaging over the whole simulation period of 10 years, we are able to calculate the HSA for rain events with a specific return period. Figure 4.12 demonstrates such an approach. During the largest daily rain event (77.2 mm) of the simulation period 23% of the catchment is active and produces surface runoff. During an average daily rain event with a monthly to quarterly return period (21.5 to 32.5 mm) only 14% of the area is active. Thereby, it
is not considered that not all areas are connected to the stream.

Figure 4.12: Surface runoff producing HSA for rain events with a specific return period based on a 10 years simulation with SMDR (1998-2007).

The runoff amount can also alter the surface connectivity. During a large storm event, it is possible that accumulated water overflows topographic barriers.

4.4.4 Environmental implications

For catchment management and the identification of HSA, the incorporation of surface connectivity is important. As Richards and Brenner (2004) and Ambroise (2004) stated, mitigation strategies should focus on locations where they are most effective, which means on connected HSA.

Simpler models combined with connectivity lead to similar predictions of HSA as physically based approaches, which are more demanding. Therefore, simpler models are useful for applications on a larger scale. Even if a DEM is the only source of information, certain risk assessment is possible. It can be used to assess the surface connectivity and since it represents some soil information, it can also be used as a basis for risk assessment. In addition, knowledge about the drainage system is useful.

Mitigation options for surface water should focus on areas prone to fast flow processes, which are connected with the river system. Options that interrupt the connectivity be-
between field sites and the river system are most promising. In this context, buffer strips for mitigating herbicide pollution by surface runoff and erosion into surface water has received much attention (cf. review of Reichenberger et al., 2007). However, their effectiveness is very variable, and the variability cannot be explained by the width of the buffer alone. Our investigations point out, that buffers are most effective, if they intercept surface connectivity. For this purpose, a slight elevation of the buffer strip could be very effective. Furthermore, large drained sink areas on agricultural fields, where surface runoff accumulates, should be avoided, since macropores can act as a close link for herbicides to the water system.

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Bibliography


Chapter 5

Conclusion and Outlook
The aim of this work was to identify risk areas for diffuse herbicide transport, so called critical source areas (CSA) or hydrological sensitive areas (HSA). The identification of these areas can help to implement effective management strategies to reduce herbicide losses to surface waters and provide a scientific, rational basis to improve agricultural policy. However, predictions of CSA and HSA locations contain uncertainties. For practical applications, these uncertainties have to be quantified and they should be reduced as much as possible. Our work focused on parameter and model structure uncertainties.

In chapter 2, we could demonstrate that hydrological modeling based on the variable source area concept can be a powerful tool to predict CSA. The prediction was based on generally available data. To understand the spatial variability of herbicide losses, it was crucial to consider the connectivity between the fields and the stream network. We demonstrated that only a limited part of our catchment is connected to the river system by the surface. Previous field studies have shown that surface runoff from those areas is responsible for the main part of herbicide pollution. We were able to assess the surface connectivity with terrain analysis tools based on a high resolution digital elevation model (DEM). Our analysis showed that a high resolution DEM is mandatory for that purpose. In contrast, a topographical analysis based on a DEM with low resolution leads to a large overestimation of the amount of surface runoff reaching the stream.

Areas that are not surface connected are not necessarily no risk areas. Surface runoff, including mobilized herbicides, from unconnected areas accumulates and infiltrates in local sink areas. A large part of the infiltration takes place through macropores. They build preferential flow paths from the soil surface into the soil layers below. If sink areas are artificially drained, macropore flow can be directly linked to the surface water system. Due to sorption and degradation, herbicide concentrations in drainage systems are expected to be smaller than in surface runoff. Nevertheless, sink areas remain potential hot spots for herbicide pollution.

In chapter 3, we have shown that our prior prediction involves large uncertainties, since the knowledge of the model parameters is fairly coarse. Model parameters were not the only sources of uncertainty. In our case study, we could demonstrate the important influence of the model structure on the prediction uncertainty. To reduce the uncertainties, additional information was necessary. We used the river discharge because this is generally the only available data source.

To calculate the prediction uncertainties, we applied a Bayesian inference approach. In the Bayesian approach, our prior knowledge is combined with the additional river discharge data to incorporate our entire process understanding. The incorporation of
prior knowledge also helped to overcome the problem of parameter identification. Most importantly, we were also able to account for uncertainty in input and model structure with a carefully chosen likelihood function.

Measurement errors are larger at higher discharge and deficits in the model structure lead to autocorrelation in the errors. To account for that, we combined the likelihood function of the deterministic model with an autoregressive error model and transformed the model results and the measured data with a Box-Cox transformation.

By incorporating different error sources, the uncertainty analysis yielded realistic error bands for the discharge prediction. In contrast, the uncertainty range did not capture the measured data if parameter uncertainty was exclusively considered.

The uncertainty of parameters with a great influence on the model results and a high prior uncertainty were reduced based on discharge data. The spatial extent of CSA was only constrained to a limited degree. The residual analysis demonstrated that this error model could largely improve the statistical assumptions of the inference process. However, the analysis still showed some systematic deviation, which pointed to deficits in the model structure.

Through improvements in the model structure the agreement between the residuals (and innovations) and the statistical assumptions could be largely improved. Furthermore, the improvement nearly halved the model structure bias. The model improvement had also important implications on the prediction of CSA. Information from the discharge combined with the improved model structure constrained the uncertainties in the CSA predictions substantially.

A comparison between the simulation results of the original (chapter 2 and 3) and the improved model (chapter 3) showed remarkable differences in the spatial prediction despite fairly similar discharge prediction. This demonstrates that an accurate discharge prediction is certainly mandatory but no guarantee for an accurate prediction of the spatial distribution. However, both models agreed in predicting CSA at certain locations and basically differed only in the extent of the CSA around these “core” areas or hot spots.

The limitation of the Bayesian approach is its high computational demand characteristic for all Markov chain Monte Carlo methods. The disadvantage of the applied error model is that it only accounts for additional error sources in the calibrated discharge. The uncertainties for the CSA prediction may be underestimated.

The comparison of different competing models in chapter 4 showed that their spatial predictions of risk areas agreed fairly well. Approaches relaying on soil data or on
topography lead to similar HSA. This indicates that topography is reflected in the soil distribution in this landscape.

However, the analysis again revealed the importance of the connectivity for the prediction of CSA. The connectivity, especially at the small scale, had not yet been explicitly implemented in prediction tools for CSA.

**Practical recommendations**

For the identification of CSA, we recommend the combination of approaches which assess the vulnerability for hydrological fast flow processes with information about the connectivity.

A topographic analysis can be a very useful starting point to predict the spatial distribution of CSA:

First, the surface connectivity can be assessed based on a terrain analysis with a DEM. For that purpose a high-resolution DEM is mandatory, since small scale structures can be crucial. Without them, the surface connected area is largely overestimated. Thanks to Airborne-Laser-Scanning, such high-resolution data are becoming more frequently available.

Secondly, the topography provides, in topographic influenced areas, knowledge about the spatial extent of areas prone to saturation, where fast flow processes are frequently initiated. The combination of this information gives a first useful assessment of CSA.

Thirdly, sink areas can also be identified on high-resolution DEMs. Artificially drained, such sink areas can be additional hot spots for herbicide pollution.

For practical application, an analysis based on a DEM is very handy, since topography is relatively easy to measure at a larger scale. DEM investigations are also applicable at a larger scale where the use of more demanding physically based models is restricted.

Soil data can further improve the prediction of fast flow producing areas which get more important as a catchment is less influenced by the surface topography. Knowledge about the drainage system is needed to estimate the risk of sink areas.

Even though the uncertainties in the prediction of CSA locations are relatively high, different approaches investigated result in similar predictions. On the one hand, they primarily agree about some “core” areas, mainly placed directly along the stream. On the other hand, there are also large parts which are seen as non critical in most approaches. These agreements by the conceptually different spatial prediction also in-
crease our confidence in the reliability of the CSA predictions.

Mitigation options for surface water should focus on areas prone to fast flow processes, which are connected with the river system. Options that interrupt the connectivity between field sites and the river system are most promising. In this context, buffer strips that stop surface runoff are often used. To increase the efficiency a slight elevation of the buffers could be very effective. Intercepting the drain flow from sinks is more difficult. Stopping surface runoff from running into sink areas or reduced cultivations could be options.

**Outlook**

Besides erosion induced by surface runoff, it is also possible that rainfall detaches soil particles from the soil surface and leads to surface sealing, which initiates Hortonian overland flow. This possible transport process for herbicide pollution of surface water is not incorporated in our investigated approaches to predict CSA. In future approaches, this process needs further consideration.

Validation of CSA remains a difficult task. Spatially distributed measurements of herbicide pollution are very time demanding and costly. To improve predictions of CSA locations and decreased uncertainties better validation data are mandatory. Calibrating models only on discharge data probably leads to higher Nash and Sutcliffe efficiencies. However, by incorporating additional data criteria into the calibration, a better overall performance may be achieved. Examples of promising data types are qualitative information like hydromorphological features from soil maps or remote sensing data. However, the spatial resolution (vertical and horizontal) of remote sensing methods is still limited.

The next step for assessing the predictability of CSA locations would be the validation of our prediction tools in other catchments on a larger scale.
Chapter 5. Conclusion and Outlook
Acknowledgements

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Education and Studies

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1990-1997  Secondary School I/II and Federal Maturity Certificate Type C, Alpenquai (Lucerne/Switzerland)
1984-1990  Primary School at Reussbühl and Kriens (Switzerland)

Professional Experience

2004      Research visit at the Oregon State University (US) in the group of Prof. Jeff McDonnell
2004      Research assistant at Eawag in Duebendorf at the Department of System Analysis, Integrated Assessment and Modelling
2003      Research assistant at Eawag in Kastanienbaum at the Department of Applied Aquatic Ecology
2000-2002 Practical work and part-time employment at the engineering office Jungo AG in Zurich
2000-2001 Teaching assistant at ETH Zurich in System Analysis (Prof. Dieter Imboden)