# MANAGEMENT SUPPORT BY OPTIMIZATION-BASED TRADE-OFF ANALYSIS – THE EXAMPLE OF BIODIESEL CROP PRODUCTION

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**SUMMARY**

Modeling in decision support applications has often been used to compare outcomes between alternative scenarios of decision options. The introduction of optimization methods enable the comparison of a very large number of scenarios that can be used to construct an approximation of Pareto optimal trade-offs among competing objectives. These represent the best compromise solutions that are available to the stakeholders. We show for the example of biodiesel crop production how such an optimization approach can be used to identify a set of potential solutions. We specified the separate objectives of biodiesel crop production, food and fodder production, water quality and minimum discharge, and searched for the best trade-offs among them using a relative recent optimization method. The analysis was based on an integrated river basin model (SWAT) and a multi-objective genetic algorithm (NSGA-II), and was set in the Parthe catchment in Central Germany. To ease communication with stakeholders and decision makers, we identified clusters in the results through use of a self organizing map approach. The clusters represent solutions of similar management strategies for the watershed, from which decision makers and stakeholders can select suitable compromise solutions. The effects of increased biodiesel crop production on the other objectives were mainly triggered by the share of silage corn and sugar beets in the crop rotations. Generally speaking, negative effects on low flow caused by increased biodiesel crop production in the region could be avoided by a shift from silage corn to sugar beets or a reduction of total crop yields. Nitrate concentrations were more sensitive to total crop yield by bioenergy and food and fodder crops.

**Keywords**: River Basin Management, water quality, bioenergy, land use, genetic algorithm, crop rotation schemes, self organizing map, optimization, trade-offs

**ZUSAMMENFASSUNG**

Simulationen im Umweltbereich werden oftmals eingesetzt um die Ergebnisse unterschiedlicher Szenarien miteinander zu vergleichen. Mithilfe von Optimierungsansätzen lassen sich darüber hinaus potentielle Managementmaßnahmen in sehr hoher Zahl vergleichen. Auf Grundlage dieses Vergleiches lassen sich dann Pareto-optimale Zielkonflikte zwischen den einzelnen Zielen abschätzen. Pareto-optimale Lösungen stellen Kompromisslösungen hinsichtlich der unterschiedlichen Zielerreichungsgrade dar und können von Entscheidungsträgern und Interessensvertreten verwendet werden, um den für sie bevorzugten Lösungsbereich zu identifizieren. Wir zeigen in der vorliegenden Arbeit am Beispiel der Biodieselpflanzenproduktion optimale Lösungen abgeleitet werden können.

Als Zieldimensionen fanden dabei Mindestabfluss, Wasserqualität, sowie der Ertrag von Nahrungs- und Futterpflanzen sowie der Ertrag von Energiepflanzen für die Biodieselproduktion Verwendung. Hinsichtlich der Energiepflanzen wurde nur Raps eingesetzt, da dieser hinsichtlich Biodieselproduktion in Deutschland die dominante Anbaufrucht ist. Die Optimierung verwendet ein Einzugsgebietsmodell (SWAT) zusammen mit einem mehrdimensionalen genetischen Algorithmus (NSGA-II). Die Analysen wurden im Einzugsgebiet der Parthe in Sachsen durchgeführt. Um die Kommunikation mit Entscheidungsträgern und Interessensvertretern zu vereinfachen wurden die Ergebnisse mithilfe einer self-organizing map geclustert. Die abgeleiteten Cluster repräsentieren dabei Managementstrategien, die ähnlich hinsichtlich der eingesetzten Fruchtarten und der Wasserqualität und des Mindestabflusses sind. Steigende Bioenergieproduktion bietet nach unseren Simulationen durchaus Anpassungspotential. Insbesondere die Anteile von Silage Mais und Zuckerrüben in den Fruchtfolgen hatten großen Einfluss hinsichtlich Mindestabfluss und Wasserqualität. Negative Effekte auf den Mindestabfluss durch steigenden Rapsanbau konnten durch eine Verschiebung von Silage Mais hin zu Zuckerrüben oder eine generelle Reduktion der Nahrungs-und Futtermittelproduktion aufgefangen werden. Für die Wasserqualität hinsichtlich Nitratkonzentrationen spielte weniger das Ausmaß des Rapsanbaus als die gesamte Pflanzenproduktion im Gebiet die entscheidende Rolle.

Schlüsselworte: Einzugsgebietsmanagement, Wasserqualität, Bioenergiepflanzenproduktion, Landnutzung, Genetischer Algorithmus, Fruchtfolgen, Self organizing maps, Optimierung, Zielkonflikte

# 1 INTRODUCTION

Decision makers in environmental management are oftentimes confronted with complex questions in which the outcomes of management strategies and the associated trade-offs among different objectives cannot easily be foreseen. Simulation models play an important role in informing decision makers about the likely outcomes of management options, but the range of potential options is typically rather large. Therefore, efficient ways to identify suitable options are needed.

At the regional planning scale, the large number of conflicts in environmental decision making can be attributed to the fact that land is a limited resource, but is used for a number of often conflicting purposes. The importance of the concept of multi-functionality of landscapes for solving resource use conflicts was identified early (Seppelt et al., 2009). Strategies that maximize a single function, such as productivity, can be expected to feedback negatively on several other ecosystem functions and services with consequences on human well-being. Instead, trade-offs need to be taken into account to reconcile requirements and demands, which are measured by environmental, economic and social indicators.

The increasing demand for biofuels is challenging to environmental managers and planners, since it involves a number of trade-offs with a large number of environmental goods and services. The Renewable Energy Roadmap of the European Union (European Commission, 2007) sets the goals of a 20% share of European energy consumption by 2020 and a binding 10% share of renewable energy use in the fuel sector. Within that framework, the member states define their own national targets. Germany aims at increasing its share of energy from renewable resources in final consumption from 5.8% in 2005 to 18% in 2020 (Fräss-Ehrfeld, 2009). Supported by tax exemptions and quota obligations, the use of biofuels in the German transport sector has already increased from 3.8% in 2005 to 7% in 2007 (German Environmental Ministery, 2009). In 2008, the largest share (69%) of renewable energy production in Germany was from biomass (German Environmental Ministery, 2009).

While the target for bioenergy production has already been set by legislation, quantitative evaluation of the costs and benefits of bioenergy production are only beginning. At present, first generation bioenergy crops compete with food and fodder production on arable land. Negative effects of increasing bioenergy production are expected (Fargione et al., 2010; Gasparatos et al., 2011; Tilman et al., 2009), including effects on biodiversity (Fitzherbert et al., 2008; Fletcher et al., 2010), biological control (Landis et al., 2008) and water (P. Gerbens-Leenes et al., 2009; W. Gerbens-Leenes et al., 2009; Martin, 2011; Yeh and Studies, 2011). However, quantification of the trade-offs among objectives in bioenergy crop production is problematic, and the number of studies that have been published on that topic is limited. Usually, trade-offs have been quantified based on a comparison of plausible scenarios (e.g. Donner and Kucharik, 2008; Meehan et al., 2010; Engel et al., 2012), but do not consider whether the reported trade-offs are optimal or not. Therefore, the solution found might be sub-optimal with respect to other land management options that have not been included in the limited set of scenario options. Decisions based on those trade-offs are therefore likely to lead to sub-optimal outcomes as well. The use of a multi-objective optimization of land use will help to overcome that problem (Seppelt et al., 2013).

Optimization algorithms have been widely used in environmental modeling. An overview about the many different applications of evolutionary algorithms in water related research is provided by Reed et al. (2013) and Nicklow et al. (2010). A number of approaches have been based on economic optimization models with respect to land use, such as linear programming, compromise programming or goal programming. For water related assessments, many studies have linked economic optimization with simulation models of groundwater leaching to specify groundwater quality/farm income trade-offs. Whittaker et al (2003) analyzed the effect of an incentive policy on nutrient runoff from agricultural production in a large basin using data envelopment analysis models linked to SWAT. Meyer et al. (2009)used SWAT and GIS models together with goal programming to identify trade-offs between farm income based on agricultural production and nitrogen leaching. Darradi et al. (2012) used a comparable tool chain to study the trade-offs between water yields, sediment loads, nitrogen concentrations and crop yields. Seppelt and Voinov (2002, 2003) as well as Seppelt and Lautenbach (2010) used single-objective genetic algorithms to optimize land use patterns with respect to costs and benefits of the different land use types under varying shadow prices for nitrate leaching. Klein et al. (2013) used a genetic algorithm together with a weighting approach to optimize adaptation strategies for agricultural land under climate change. Polasky et al. (2008) used a heuristic search algorithm to study trade-offs between biodiversity and economic returns of land use. Holzkämper et al. (2006) as well as Holzkämper and Seppelt (2007) optimized land use with respect to habitat requirements of birds and the value of arable land using a single-objective genetic algorithm together with weighing schemes for the different objectives. Rabotyagov et al. (2010) employed SWAT together with the multi-objective genetic algorithm SPEA2 (Zitzler, 1999) to study trade-offs between costs and nutrient emissions. The model chain that we employed here, SWAT and NSGA-II, has been applied before in different contexts and with different aims. Maringanti et al.(2009) and Rodriguez et al. (2011) used SWAT and NSGA-II to identify the spatial allocation of best management practices (combinations of pasture management, buffer zones, and poultry litter application practices). Selection and placement of these best management practices were analyzed under different cost solutions. Panagopoulos et al. (2012) used SWAT and NSGA-II to optimize the placement of fifty different best management practices (livestock, crop, soil and nutrient application management in alfalfa, corn and pastureland fields) with respect to cost, phosphorus and nitrogen emissions. Whittaker (2005) applied the model chain for the analysis of trade-offs between agriculture and salmon habitat protection. In this study, alternative policies (command and control regulation and tax incentives) to reduce non-point emissions of nitrogen from agriculture were evaluated with respect to the environmental efficiency and effects on profits were compared. Groot et al. (2007) used an optimization approach related to NSGA-II to study the trade-offs between plant species number, nitrogen loss, and landscape value. The study used land-use intensity and hedgerow presence as control variables.

The goal of the study was the quantification of functional trade-offs based on such a multi-objective land use optimization. Our goal was an a posteriori decision tool where decision maker preferences for alternatives are expressed after non-dominated or Pareto-optimal alternatives have been identified. All solutions are initially assumed to have equal preference during the search process. The preferences of a decision maker are expressed in a later step during the exploration of trade-offs and the selection of design solutions. We considered trade-offs between bioenergy as well as food and fodder crop production with regard to water quality and water quantity in a meso-scale agricultural basin. Our research product was information on biophysical trade-offs at the regional scale for stakeholders. We focused on rapeseed as a bioenergy crop, which is by far the most important source of biodiesel in the EU, especially in Germany (Deutscher Bundestag, 2012; Spencer et al., 2011). The work presented here builds on the analysis of Strauch (2008) and Strauch et al. (2010), who used a scenario approach to study the effects of climate change and different bioenergy production options in the Parthe basin. The work has been extended (Lautenbach et al., 2012) to quantify and map the nitrogen retention ecosystem service in the case study region. A first methodological work on the analysis of the trade-offs of biodiesel production in the watershed have been presented in Lautenbach et al. (2013). In the current study, we put our focus on the aggregation of results with respect to decision support. To simplify the communication with stakeholders, effects of an aggregation of the results based on clustering approaches were tested.

# 2 DATA AND CASE STUDY

## 2.1 CASE STUDY

The analysis took place at the Parthe basin in East Germany close to the city of Leipzig (cf. Figure 1). It is a sub-basin of the Weisse Elster catchment in the Elbe river system and drains an area of about 315km$^2$. The topography of the basin is mainly flat with elevations from 110m at the outlet up to 230m in the Southeast. Due to its location in the lee of the Harz mountains, the area is characterized by low precipitation. The mean annual precipitation at the weather station Brandis is 660mm while the mean annual potential evapotranspiration reaches 630mm. The subsurface is predominantly formed by moraine material. Bedrock is only present in the southern and eastern part of the area. The moraine sediments are between 1m and 20m thick and are covered by an approximately one meter thick layer of aeolic sand-loess material. The Parthe is a typical lowland river where runoff dynamics are characterized by high flows in spring due to snowmelt, and little rainfall and long periods of low-flows in summer with occasional storm flow events. Mean long-term flow rate of the Parthe is 0.9m$^3$ s$^{-1}$.

The region is used intensively for agriculture: about two thirds of the total basin area are used by agriculture, 15% are residential areas, additional 15% are covered by forest and about 1% by open water bodies. It has been shown that crop rotations and associated management practices have a significant effect on discharge and water quality of the Parthe (Ullrich and Volk, 2009). Changes in crop rotation due to an increasing demand for bioenergy production are therefore of concern. Building on the experience from previous studies, which incorporated input of farmers and stakeholders such as the Saxon State Agency for the Environment, Agriculture and Geology (Ullrich and Volk, 2009) and the State Agency for Flood Protection and Water Management Saxony-Anhalt, we decided to focus on four objectives: low flow, average nitrate concentration, bioenergy crop production and food and fodder crop production. Since a part of the drinking water for the city of Leipzig (~ 500,000 inhabitants) is taken from near surface groundwater connected to the river flow

(Ingenieurbüro für Grundwasser Leipzig GmbH, 1997), low-flow values during the summer months are a serious concern for the management of the Parthe River. In addition, rivers must not dry up, nor should their physical regimes significantly alter, in order to preserve the hydrological and ecological functions of the river drainage networks. Water quality, especially nitrate concentration, is a further major concern with respect to the 'good ecological status' as defined by the water framework directive of the EU.

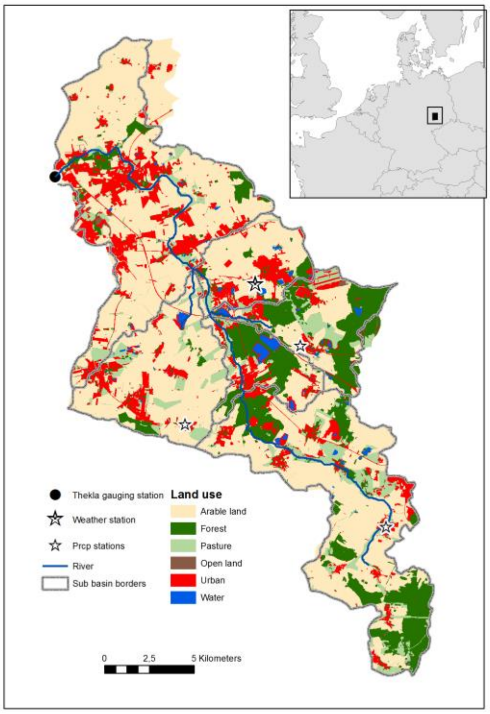


**Fig.1:** The Parthe case study region is located in Eastern Germany, close to the city of Leipzig. It is dominated by arable land with significant parts covered by forest, grassland and urban land. The weather station did also provide information on precipitation.

## 2.2 DATA

Meteorological input data came from four precipitation gauges and one climate station (cf. Figure 1). A Thiessen polygon approach was used to weight the precipitation stations. Information on discharge and water quality was provided by the Saxon State Agency for the Environment, Agriculture and Geology. We used only time series for the gauging station at the basin outlet in Thekla. Terrain information was derived from the digital elevation model of the federal state of Saxony (30x30m cell size). Soil data were derived from a digitized soil map compiled by M. Thomas-Lauckner (1:25.000). Land use data were derived from the color and infrared (CIR) biotop and land use classification of the federal state of Saxony (1992). Management practices such as crops grown, fertilizer application, and tillage operations for different land uses were gathered from district agricultural statistics and transformed into typical crop management schedules with the assistance of agronomists (Abraham, 2004). Non-point source emissions were derived based on information on existing sewage treatment plants in the basin provided by the Environmental Operating Service of the Saxon State Agency for the Environment, Agriculture and Geology. We also included data on groundwater withdrawal based on information by the local waterworks.

# 3 METHODS

## 3.1 TRADE-OFF ANALYSIS

The aim of the study was to identify functional trade-offs and to spot the effects that different crop rotations play in that system. The base of the analysis was a watershed model that has been parameterized for the conditions in the watershed. During the calibration, model parameters are adjusted to achieve a better model performance. The best fitting model parameterization was then employed inside of an optimization algorithm to find and identify the Pareto-optimal solutions which can be interpreted as functional trade-offs (cf. Figure 2). The Pareto-optimal solutions were afterwards analyzed with a clustering approach to spot patterns with respect to control variables (crop rotations) and objectives. In a last step, the model was rerun for all Pareto-optimal crop rotation allocations. This time, in addition to low flow and nitrate concentration the yields for all crops were recorded. These yields together with the low flow and nitrate concentration values were used to detect clusters in the data using a self organizing map. In addition a generalized additive model was run to detect non-linearity in the relationship between low flow and nitrate concentration and the individual crop yields.

### 3.1.1 WATERSHED MODEL

We used the Soil Water Assessment Tool (SWAT) (Arnold and Fohrer, 2005) to model the effects of different land use options on water quality and discharge. The model has been used in many studies world-wide to evaluate the impact of land use scenarios and management practices on landscape water fluxes and water quality (Gassman et al., 2007; Volk et al., 2009). SWAT is a physically-based, conceptual, continuous-time river basin model with spatially semi-distributed parameters operating on a daily time step. It was designed to simulate broader scale patterns of discharge and water quality in the spatial and temporal domain (Neitsch et al., 2005b). The model integrates all relevant processes for watershed modeling including water flow, nutrient transport and turnover, vegetation growth, land use, and water management at the sub-basin scale. It considers five different pools of nitrogen in the soils (Neitsch et al., 2005b): two inorganic (ammonium and nitrate) and three organic (fresh organic nitrogen and active and stable organic nitrogen). Nitrogen is added to the soil by fertilizer, manure or residue application, fixation by bacteria, and atmospheric deposition. Nitrogen losses occur by plant uptake, leaching, volatilization, denitrification and erosion.

The area of the case study watershed was divided into 6 sub-basins based on a digital elevation map. SWAT uses the concept of hydrological response units (HRU) to further subdivide the sub-basins. The HRUs contain similar terrain, similar soil characteristics, and similar land use. In consequence, SWAT is not only spatially explicit at the level of sub-basins, but accounts also for heterogeneous landscape characteristics in form of the HRUs. For our application, the area was divided into 53 HRUs. The water balance for each HRU is represented by four storages that consist of snow, soil profile, shallow aquifer, and deep aquifer. The soil profile can be subdivided into as many as ten soil layers - we used seven soil types with up to five soil layers in our case study. Soil water processes include evaporation, surface runoff, infiltration, plant uptake, lateral flow, and percolation to lower layers. The surface runoff from daily rainfall is estimated with a modification of the SCS curve number method (Arnold and Allen, 1996; Neitsch et al., 2005b). The different runoff components and matter fluxes are routed to the sub-basin outlets, where modeled and observed discharge as well as water quality data can be compared.

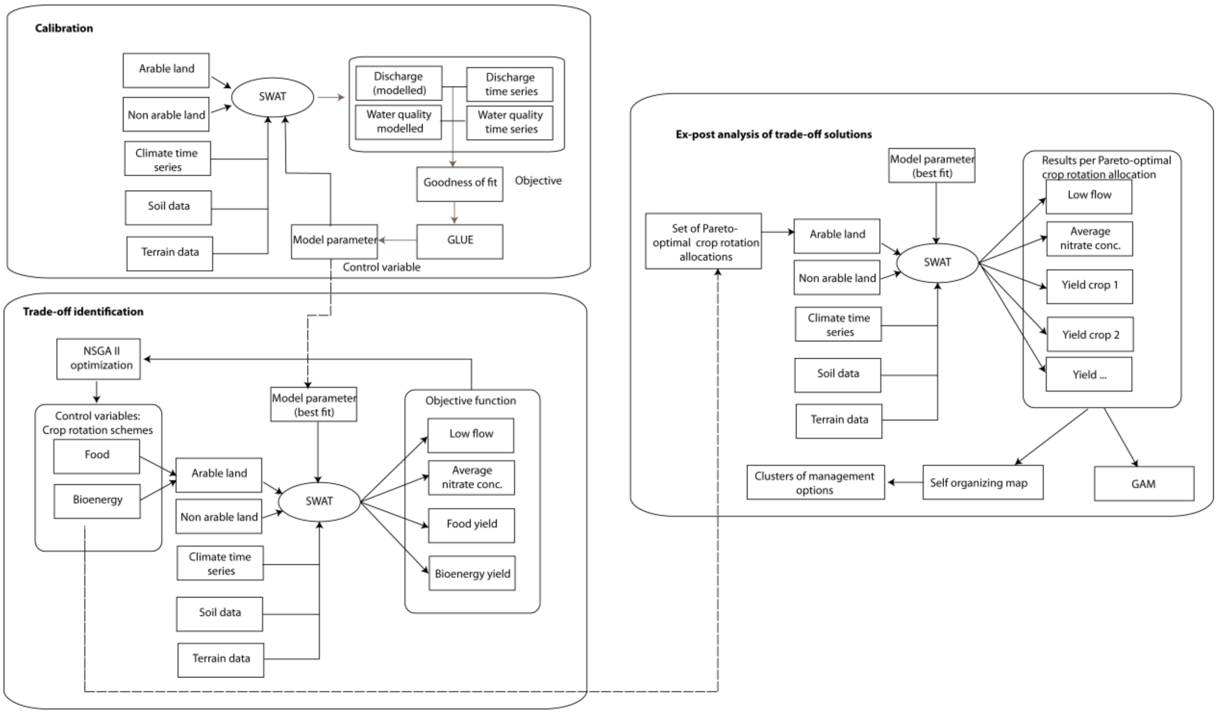


**Fig.2:** Flowchart of the analysis. First, the model was calibrated against measured discharge and water quality data. During the calibration, model parameters are adjusted to achieve a better fit (for details see text). The best fitting model parameterization was then used to identify the Pareto-optimal allocations of crop rotation schemes to the 13 agricultural HRUs. The optimization algorithm searches for the best solutions with respect to the four dimensional objective function by optimizing the allocation of crop rotation schemes on arable land. The distribution of non-arable land is not modified during the optimization neither are other input variables like climate time series, soil data or terrain. In the last step, the model was rerun for all Pareto-optimal crop rotation allocations. This time, in addition to low flow and nitrate concentration the yields for all crops were recorded. These yields together with the low flow and nitrate concentration values were used to detect clusters in the data using a self organizing map. In addition a generalized additive model was run to detect non-linearity in the relationship between low flow and nitrate concentration and the individual crop yields.

### 3.1.2 MODEL CALIBRATION AND VALIDATION

The model was calibrated for monthly streamflow and nitrate load at gauge Thekla using the Generalized Likelihood Uncertainty Estimation (GLUE) method (Beven and Binley, 1992). Calibration period was from 1992 to 2002, in which data on nitrate were only available in sufficient quality from 1999 to 2002. Based on an initial sensitivity analysis and on previous experience with the calibration of the model, a set of parameters was selected for use in calibration. Calibration ranges and default values of the other parameters were specified using recommendations given by the model developers (Neitsch et al., 2005a). The model was calibrated simultaneously for both discharge and nitrogen load. Finally, crop yields were checked for plausibility based on information provided by the agricultural statistics for the NUTS 4 level.

The GLUE analysis accounts for equifinality of parameter sets and consisted of the following three steps: (i) The parameter space was randomly sampled resulting in 15,000 parameter sets. Nash-Sutcliff efficiency (NSE) was used as a "generalized likelihood measure", calculated for the joined output time series of streamflow and nitrate load. NSE values range from minus infinity to 1, where higher values represent a better goodness of fit. Following the nomenclature used in the application of GLUE, parameter sets that resulted in a NSE higher than 0.45 were considered as "behavioral", all others as "non-behavioral", (ii) A likelihood weight $w_i$ was assigned to each "behavioral" parameter set $i$ according to equation 1, where N is the total number of "behavioral" parameter sets, (iii) Finally, the 95 % prediction uncertainty (95 PPU) interval was calculated based on the cumulative distribution realized from the "behavioral" parameter sets sorted according to the weights $w_i$.

$$w_i = \frac{L(\Theta_i)}{\sum_{k=1}^{N} L(\Theta_k)} \qquad (1)$$

Due to the few time series where both nitrate and streamflow data were available, the model was validated only for streamflow (for the period from 2003 to 2007). Overall, model performance was satisfactory with Nash-Sutcliff efficiency values of 0.52 (calibration) and 0.70 (validation) for predicting streamflow and 0.67 for predicting nitrate load. In the trade-off analysis, we used only the best selected model to assess the effects of the different management schemes.

### 3.1.3 CONTROL VARIABLES AND OBJECTIVE FUNCTION

The use of an optimization approach requires that both control variables (which specify the range of management options) and objectives (which specify how the result of different management options should be compared) need to be defined. The control variables were defined as a set of predefined crop rotations with associated management practices. During the optimization run different spatial allocations of the crop rotations were tested.

Crop rotations and associated management practices such as fertilization or the date of sowing are important parameters of the SWAT model. Crop rotation schemes followed Abraham (2004), who defined typical crops rotation schemes for the Weiße Elster watershed, where the Parthe is a sub-basin (Rode et al., 2008). We modified these schemes to fit our requirements by using specific crop rotation rules (Freyer, 2003) that specify, for example, that rapeseed can only be farmed every third year due to pest pressure by nematodes. These crop rotations were used during the calibration and validation of the model.

The range of management options during the optimization was defined by a fixed set of 26 crop rotations. These 26 crop rotations were derived based on the basis crop rotations used during model set up.  We derived crop rotations representing only food and fodder production by eliminating rapeseed from the crop rotations. For biodiesel crop rotations, we increased the share of rapeseed up to 30 % in the crop rotations. Roughly 60% of the catchment area was covered by arable land, represented in the model by 13 of the 53 HRUs. There was no economic or biophysical reason for other land use allocations. Therefore, we decided to remain forest, pasture, water and residential areas in their current use, and to modify only the crop rotation schemes on existing farmland areas – i.e. only these 13 HRUs were considered in the optimization approach. Each crop rotation was tagged with a unique ID. This ID was then used to map crop rotation schemes to the HRUs in the genetic algorithm. Each crop rotation scheme was associated with a set of management actions such as tillage and fertilizer application. These management schemes reflect current practice in the case study region.

### 3.1.4 OBJECTIVE FUNCTION

We specified four objective functions to be maximized in the optimization:

1. maximize harvested yield of food crops used (yield food and fodder), measured in tons dry weight, summed over the whole period,
2. maximize harvested yield for rapeseed (yield bioenergy) in tons dry weight, summed over the whole period,
3. maximize discharge under low flow conditions (low flow), measured as the 5 percentile of discharge at the gauging station Thekla in m3 per second

4. minimize the average NO3- concentration at the gauging station Thekla in mg N per liter (nitrate concentration).

The trade-offs were quantified in biophysical units. In other words we were interested in how much minimum discharge and nitrate concentration would change with changing crop rotations. The specification of objectives was done with respect to the research question, data availability and the complexity of the optimization problem. Increasing the number of dimensions of the objective function amplifies the computational effort. Optimization in four dimensions is almost always successful using the NSGA-II algorithm, and the computation time was reasonable given the available computational resources. Low flow conditions were considered important since they indicate the potential ground water withdrawal and the ecological conditions. Average nitrate concentration was selected, since nitrogen is a major concern with respect to water quality in the region. Data availability for phosphorus, as the other important water quality component, is limited and was therefore not used in the objective function.  The analysis was motivated by increasing demand for biodiesel crop production, so we included yield for rapeseed in an objective function. Since bioenergy crop production is in direct competition with food and fodder production, food and fodder yield was chosen as fourth objective. To exclude the effects of initial conditions on the objectives, we used a five year long burn-in period. During the burn-in period model results were not evaluated for the calculation of the objectives.

### 3.1.5 OPTIMIZATION ALGORITHM

Since the shape of the objective function cannot be assumed as smooth or differentiable in our application, gradient approaches such as quasi-Newton (Byrd et al., 1995; Fletcher and Reeves, 1964; Nocedal and Wright, 1999) cannot be used. Instead, gradient free methods such as evolutionary algorithms (Goldberg, 1989) or simulated annealing (Kirkpatrick et al., 1983) are applicable as optimization approaches for such problems.

We used the non-dominated sorting genetic algorithm NSGA-II (Deb, 2001; Deb et al., 2002) for the optimization of our four-dimensional objective function. Genetic algorithms code the parameters to be optimized in a genome and evaluate the fitness of an individual (which carries one genome) based on an objective function. A number of individuals form a population from which individuals are selected for mating. The probability of mating depends on the fitness of the individual, which is measured by the values of the objective function. Mating is performed by crossover operators, which randomly combine the genomes of the two mating partners. In addition, mutation operators randomly change the genome of the offspring, which increases the search space. While there is no guarantee that an optimum solution is found, genetic algorithms are known to find close to optimal solutions.

The genome consisted of the list of the crop rotation schemes applied to the agricultural HRUs. Since our model setup consisted of 13 agricultural HRUs, the genome was defined as an array of 13 integers – each integer representing a crop rotation from the set of crop rotations available. The initial population is created by assigning crop rotations from the set of available crop rotation to the HRUs. To speed-up the optimization process, we forced genomes which consist of a single crop rotations scheme for each of the HRUs into the initial population. If two individuals are selected for mating, crossover is performed such that the arrays of both parents are split at a randomly chosen position and the four parts are recombined. Since the objective function is 4-dimensional, the individuals are assigned ranks based on a non-dominated sorting scheme: an individual is dominated by another individual if the other individual has a better fitness value in one dimension of the objective function, while having the same or better fitness value in all the other dimensions (cf. Figure 3). Each individual gets a score based on the number of individuals that dominate it. All individuals that have the same number of dominating individuals are said to belong to one front ($F_i$).

The final outer-most front defines the Pareto front. For each individual on that front, any one objective cannot be improved without losing some quantity of the other objectives – this describes the trade-offs between the objectives.

Since one is interested in a Pareto front estimate that approximates the complete Pareto set, a “crowding distance” is defined which puts selection pressure on the algorithm to select individuals from the feasible range of the Pareto set. Crowding distance refers to the search space around the individual that is not occupied by another individual in the population. If the number of individuals on the Pareto front is larger than the predefined size N, individuals are selected based on their crowding distance. Individuals that are close together will be removed from the population to allow for a large spread of the individuals in the objective space. The crowding distance is also used during the selection of individuals, which are allowed to mate. We used tournament selection, where an individual wins the tournament with another randomly chosen individual if it is on a more outside front or, - if the front is the same - if it has a greater crowding distance than its opponent.

Genetic algorithms and other optimization approaches cannot guarantee that they find the optimal solution. Instead, they provide an approximation of the true optimal solution. Further, genetic algorithms and related optimization algorithms are non-deterministic: different random seeds are likely to lead to different approximations. We followed the recommendations given by Reed et al. (2013) and Nicklow et al. (2010) and used ten different optimization runs with different random seeds. The functional relationships identified by the different runs were similar but the spread of the non-dominated solutions differed. Therefore, we pooled the solutions of all ten runs and used the approach of epsilon dominance (Laumanns et al., 2002) to select a manageable subset of solutions which captures the main shape of the Pareto frontier.

ε -dominance extends the concept of dominance towards the concept of approximate domination (Laumanns et al., 2002):

Let $f,g \in \Re^{+m}$.

Then $f$ is said to ε -dominate $g$ for some $\varepsilon > 0$, if for all $i \in \{1,...m\}$ $(1+\varepsilon)* f_i \geq g_i$.

The application of the ε -dominance leads to ε -approximate Pareto set which should cover the most important characteristics of the Pareto set with a reduced and therefore more manageable number of solutions. We defined epsilon by the standardized range of the four objectives. An epsilon value of 1.5% seemed to lead to the best compromise between number of solutions and level of details.

The optimization process of each of the optimization runs was terminated based on the number of generations, where the number of generations was based on pilot simulations. Other parameters of the genetic algorithm such as the mutation rate and the population size were also selected based on a couple of pilot simulations. Given constraints on the high performance computer cluster, we aimed at a population size and number of generations that allowed the computation in 48 hours using 36 CPUs in parallel. Our simulations ran with a population size of 360 individuals and terminated after 200 generations. The implementation of the algorithm was based on the ecspy (Evolutionary Computations in Python, http://code.google.com/p/ecspy/) library, which was parallelized using the mpi4py library for Python 2.7 (http://mpi4py.scipy.org/).

### 3.1.6 POST-PROCESSING OF THE PARETO-OPTIMAL SOLUTIONS

Communication of results of a multi-objective optimization is an important but non-trivial issue especially in high dimensional objective and or design/decision spaces. Visualization of results has been identified as a key topic (Kollat and Reed, 2007). To simplify the complex shape of the Pareto frontier we searched for clusters in the non-dominated solutions. We employed a self organizing map approach (Kohonen, 2008) for that purpose. A self organizing map can be thought of as a constrained version of K-means clustering which organizes the cluster representatives in a two-dimensional coordinate system (Hastie et al., 2009). Distance in that two-dimensional coordinate system reflects similarity in the high dimensional feature space as well.

The clustering was based on the crop specific yields for each solution together with the low flow and the average nitrate concentration. Thereby, we include more management specific details in the cluster formation which should provide useful information for decision makers. Prior to the clustering we normalized all variables by scaling them to zero mean and unit variance. To allow an easier interpretation of the cluster centers (the code vectors in the jargon of self organizing maps) we back-transformed the values with respect to variance, but kept the centering of the variables. Before applying a self-organizing map approach to the data objects, a decision about the topology of the map has to be made. Based on the criterion of the minimization of the quantification error (Bodt et al., 2002) a 4 by 4 topology using a hexagonal neighborhood relationship was selected. A 2 by 2 topology which led to a similar quantification error provided too few details and was therefore not considered useful for our purpose.

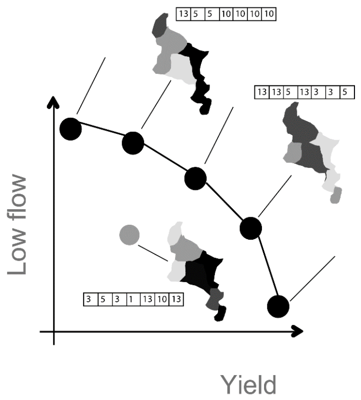


**Fig.3:** Conceptual illustration of Pareto-optimal solutions of catchment management. The graph shows a two dimensional example for a Pareto front. Each point represents the results of a SWAT model run for a different mapping of crop rotations to agricultural HRUs (represented by the genome, the array of integer values which are linked to the HRUs by position in the array– the figure is just a sketch and does not represent the HRU distribution properly). The results are condensed in two objective values, in this case total crop yield and the minimum discharge at the Thekla gauging station. The grey point is dominated by other configurations since it is possible to increase yield with the same minimum discharge and it is possible to increase minimum discharge at the same yield. The black points represent the current Pareto front. The approach can be easily transferred to higher dimensional spaces but visualizing dominated solutions in solution spaces with more than three dimensions is difficult. Note, the shape of the Pareto frontier depends on whether the different objectives are to be maximized or minimized - in the given example both objectives are to be maximized.

Since the choice of the dimensions for the clustering approach ignored the spatial configuration, the temporal placement of the crop yields and the position of the crop in the crop rotation, we ran generalized additive models (Wood, 2007) for low flow and average nitrate concentration with crop specific yields as the predictors. Generalized additive models extent generalized linear models by allowing non-linear functions for each of the predictors while maintaining additivity (James et al., 2013). To deal with non-significant effects we used penalized regression splines which shrink coefficients to zero for non-significant effects (Wood, 2007). Non-linearity in the smoothing terms can be partly interpreted as the degree to which spatially varying HRU parameters, such as soil properties and curve number coefficients, affect the results. Additionally, crop yields of same crops differ between the different crop rotations, and between years due to different weather conditions. If the HRU properties, the temporal placement of the crop yields and the position of the crop in the crop rotation have no effect, we would expect a straight line for the crop yield response.

The analysis was performed in R version 3.0.1 (R Core Team, 2013) using the packages kohonen (Wehrens and Buydens, 2007), lattice (Sarkar, 2008) and mgcv (Wood, 2007).

# 4 RESULTS

The Pareto-optimal solutions identified during the optimization step showed a complex pattern (cf. Figure 3). The four dimensional solution space contains many details that can be best seen while using an interactive visualization approach such as provided for example by GGobi (Cook and Swayn, 2007). Increasing biodiesel crop production based on rapeseed led to decreasing low flow conditions in the Pareto-optimal solutions. However, this pattern is clearly not independent from the other two objectives: the shape of the relationship between low flow and biodiesel crop production changed clearly between the different panels in Figure 3. Increasing food and fodder production had to affect biodiesel crop production since the farming area was limited. If low nitrate concentrations were to be achieved at high food and fodder yield levels, high low flow conditions were not achievable. In general, high yields for both food and fodder as well as for biodiesel crop production led to higher average nitrate concentrations.

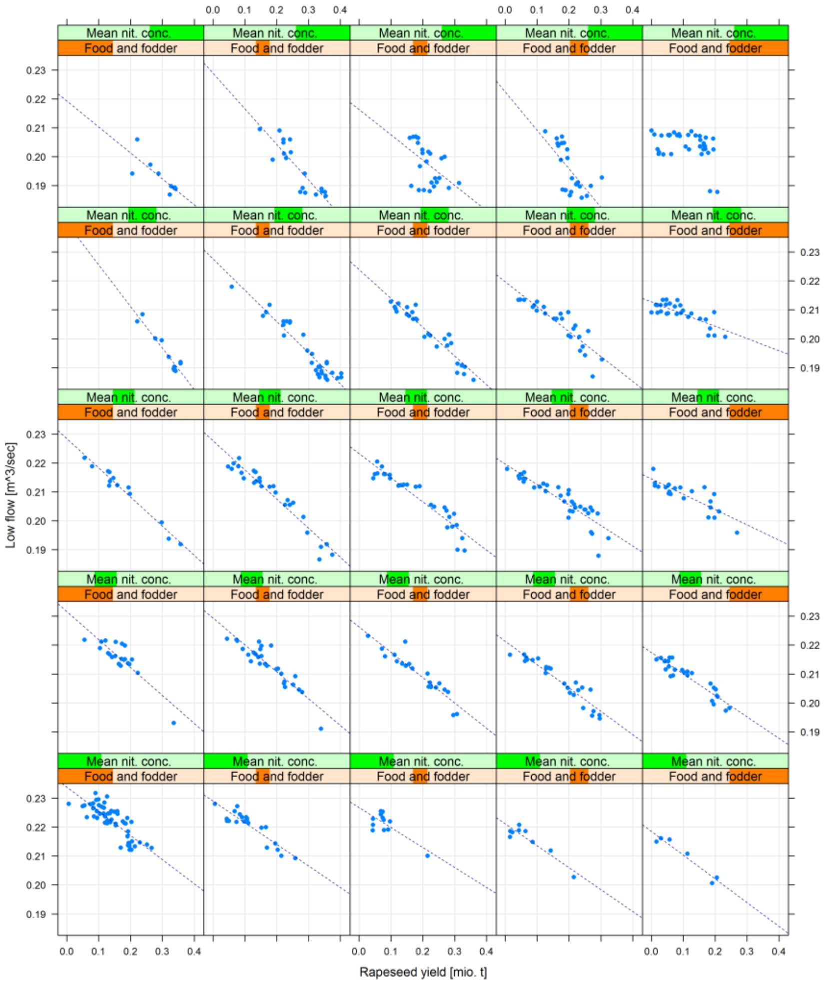


**Fig.4:** Pareto-optimal solutions in the objective space. To show the four dimensional relationships, low flow has been plotted against rapeseed yield for different levels of food and fodder yield and for different levels of average nitrate concentration. The marks in the headlines of each panel represent the range of values used for the two objectives to select the subset of points to be displayed in the current panel. Selection ranges were defined as quantiles with 15% overlap. To aid interpretation, a linear regression line has been added to the panels if the $R^2$ was higher than 0.2.

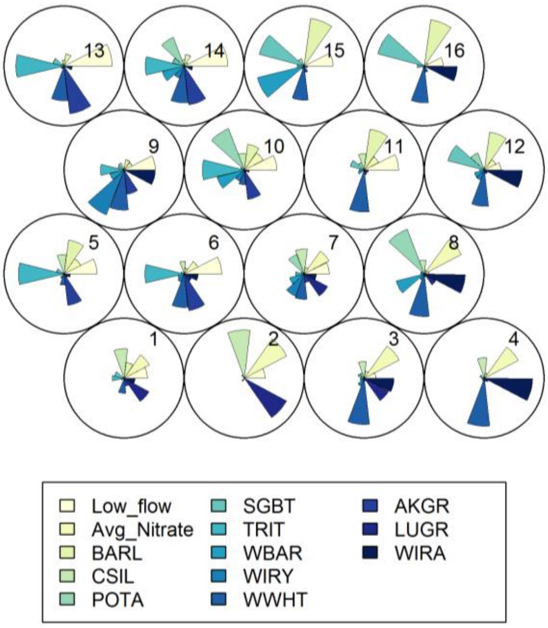


**Fig.5:** Code vector values for the clusters of management options (SOM1-SOM16). The length of the segments represents the value of the variable in the code vector (the cluster center). The values are centered and standardized to unit variance. The abbreviation represent low flow and average nitrate concentration as well as the yields of the different crops: WIRA – rapeseed, AKGR - ley, BARL - summer barley, CSIL- silage corn, LUGR - alfalfa, POTA - potatoes, SGBT - sugar beets, TRIT - triticale, WBAR - winter barley. WIRY- winter rye, WWHT - winter wheat.

The complexity of the solution space would overwhelm most stakeholders and decision makers, and complex illustrations of the results would perhaps not confirm the advantages of the method. The situation becomes even more complex if the design options (the allocation of the different crop rotations) are also considered (results not shown). The application of the self organizing map led to a much simpler representation of the solution space, and includes additional information on crop specific yields (cf. Figure 4). Interpretation should take into account the fact that the number of Pareto-optimal solutions in the different clusters was different (cf. Figure 5). Cluster 9 and 15 were clusters with a relatively low number of data objects, while cluster 13 showed the highest number of data objects mapped to it. Some clusters –namely cluster 8 and 9 - showed a higher variance than others (cf., Figure 6).

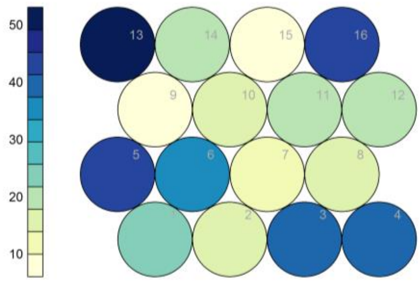


**Fig.6:** Number of Pareto-optimal solutions in each cluster.

While the clustering was done based on standardized values, interpretation was easier using the back-transformed values where crop yields are comparable (cf. Figure 7). This enables decision makers to choose between a range of options depending on their preferences for the different objectives. The clusters 13 and 14 represented environmental friendly solutions with higher than average low flows and lower than average nitrate concentrations. Both bioenergy crop production and total food and fodder production in these clusters were reduced in the optimal trade-off. In contrast, environmental unfriendly solutions were represented by the clusters 2 to 4 and 8. The other clusters represented management options in which either low flow was increased at the cost of nitrate concentration or nitrate concentration was reduced on cost of decreasing low flow conditions. Increases in food and fodder provisioning were either based on silage corn (cluster 1, 2, 4, 5, 7) or on sugar beets (cluster 12, 15 and 16), the two crop with the highest per area yield in the crop rotations. Clusters with high silage corn yields were characterized by low rapeseed yields (cluster 1, 2 and 7) while clusters with high sugar beet yields came both with increased (cluster 12 and 16) as well as with decreased (cluster 15) rapeseed yields. For cluster 15 the benefits of reducing biodiesel crop production were a strong decrease of nitrate concentration and a light increase of the low flow. With the exception of cluster 9, the trade-off for increasing bioenergy crop production was a decrease in low flow conditions. Decreased biodiesel crop production led to an increased low flow (cluster 5, 6, 10, 11, 13 and 14), if the total food and fodder yield was not increased too much (cluster 1 and 2 and 7). No clear pattern was detectable for the other crops.

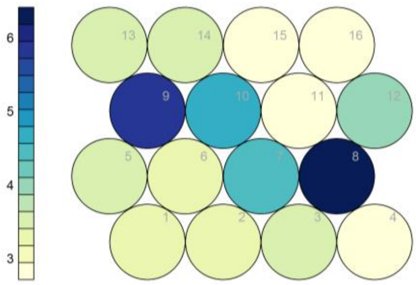


**Fig.7:** Mean distance of the Pareto-optimal solutions mapped to a cluster to the codebook vector of that cluster. The smaller the distances, the better the objects are represented by the codebook vectors.

The analysis of effects of the yields of the different crops on low flow and nitrate concentration by means of generalized additive models showed non-linearity in the effect of some crops (cf. Figure 8 and Figure 9). The goodness of fit of the generalized additive models was high (adjusted R2 of .91 and .93) – crop yields had a consistent effect on the two objectives in the Pareto-optimal solutions. For nitrate concentration non-linearity of the effect was clearest detectable for winter wheat. The other crops showed a more or less linear effect on nitrate concentration with exception for high yields. The effect of crop yields on low flow conditions showed clearer signs of non-linearity: winter wheat, potatoes and to a lesser degree silage corn, sugar beets and winter rapeseed showed non-linear effects of crop yield on low flow. Again, deviations from linearity of the effects were strongest for high yields. Effects of increasing crop yield on low flow were negative for all crops but ley while increased crop yields for all crops but winter rye and ley had a positive effect on the average nitrate concentration. One has to keep in mind that the data to which the models were fitted to represent Pareto-optimal solutions with different crop rotations used – Figure 8 and Figure 9 do not show the effect of an increase of crop yield for a single crop in isolation. If crop yield for one crop is increased, this is typically followed by an increase of crop yields of other crops in the same crop rotation and followed by a decrease in crop yields for other crops not in the crop rotation.

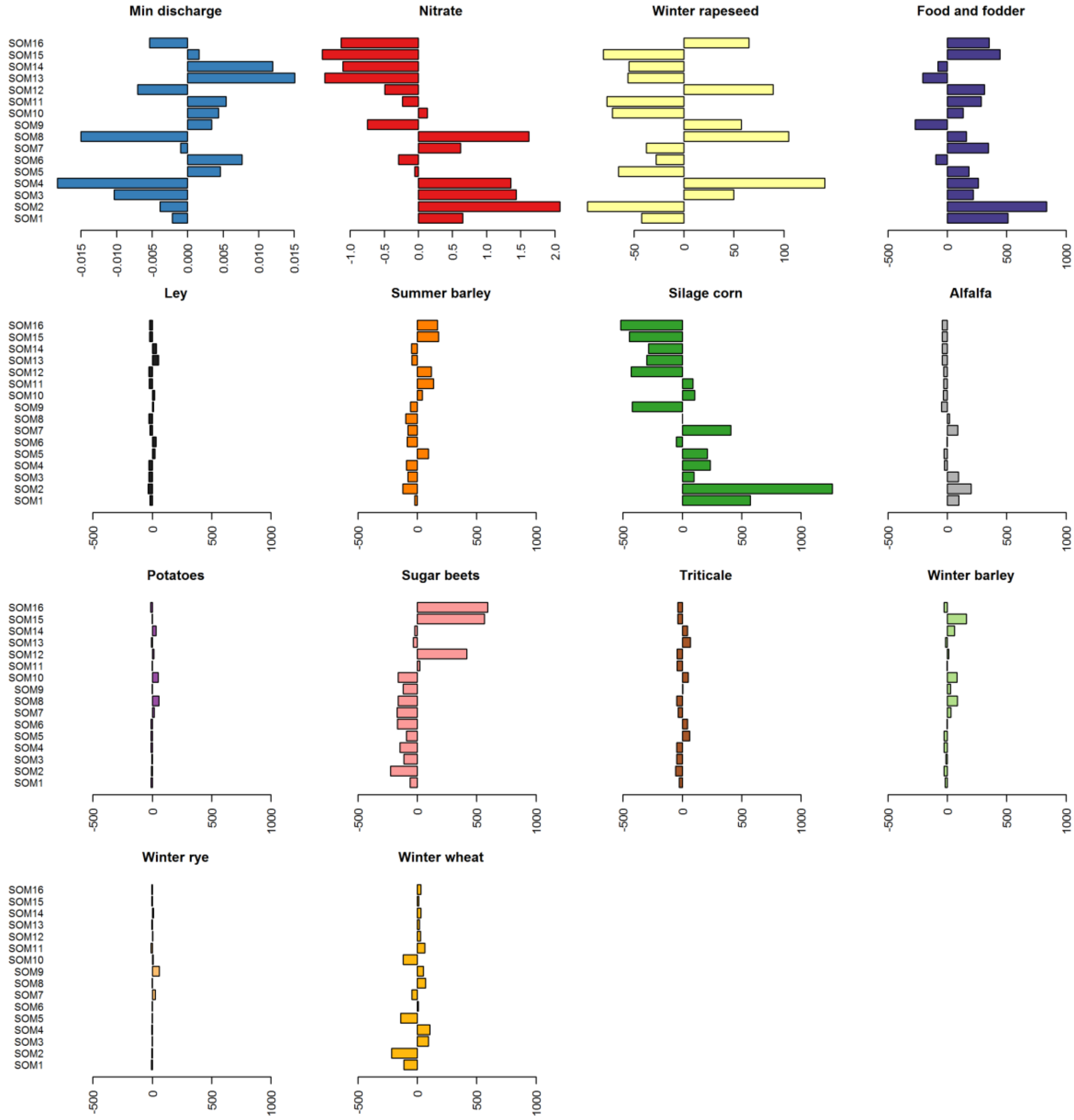


**Fig.8:** Code vector values for the clusters of management options (SOM1-SOM16). The length of the bars represents the value of the variable in the code vector (the cluster center). The values are centered but have been back transformed such that they are shown in their original scale and units ($m^3$/sec for low flow, mg N / l for nitrate concentration and yield in million tons per year for the different crops. To aid interpretation, the difference from the total sum of all food and fodder crops per cluster has been added. It should be kept in mind that the clusters contain different numbers of elements. All food and fodder crops have been plotted using the same x-axis to ease interpretation.

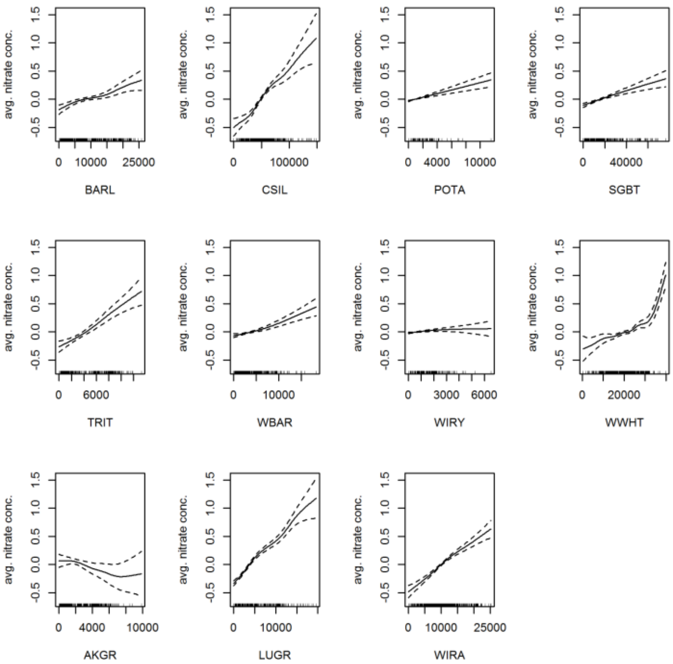


**Fig.9:** Fitted smoothing functions of a generalized additive model for average nitrate concentration. While the x-axis shows the yield of the different crops, the y-axis shows the effect of the yield of the crop on the average nitrate concentration. Dashed lines represent the 95% confidence intervals, rugs at the x-axis show the distribution of the predictor values.

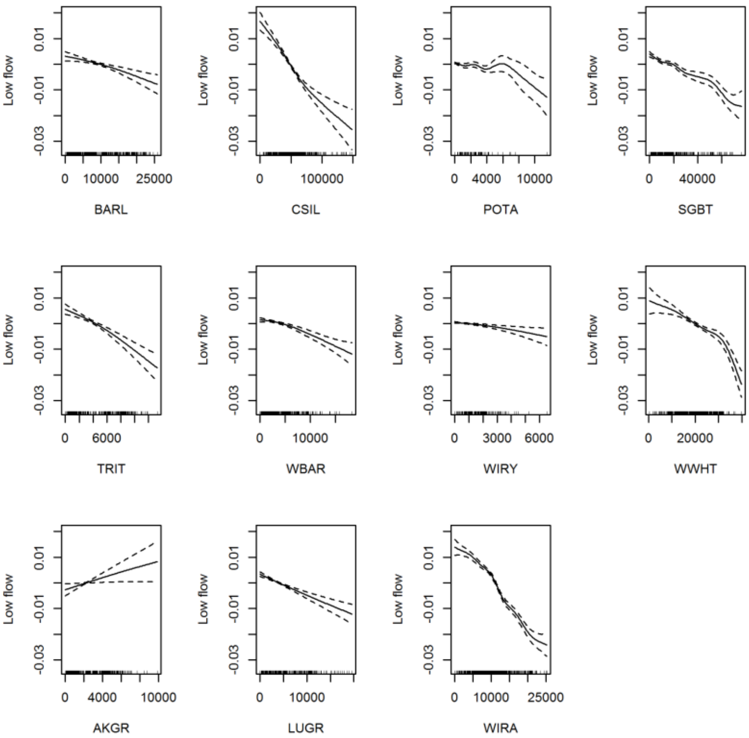


**Fig.10:** Fitted smoothing functions of a generalized additive model for low flow. While the x-axis shows the yield of the different crops, the y-axis shows the effect of the yield of the crop on the low flow. Dashed lines represent the 95% confidence intervals, rugs at the x-axis show the distribution of the predictor values.

# 5 DISCUSSION

The quality of the trade-off curve derived depends on the applicability of the simulation model, the quality of the data used for its calibration and the properties of the optimization algorithm. The clustering of results is sensitive to the selection of the clustering algorithm.

Models with a large number of parameters, such as SWAT, have to face the question of overfitting and equifinality (Beven, 2006) – if several parameter combinations led to similar model efficiency measures but lead to different model behavior, a good calibration result cannot guarantee a good representation of model behavior by the model. However, Whittaker et al. (2010) showed for SWAT that constraints provided by the model equations and the directed stream network regularize the calibration process and prevent overfitting during the calibration period. Calibration and validation results for the SWAT model were satisfying, so the results seemed reliable. It should be further taken into account that the objective values integrate over the whole simulation period and were therefore less sensitive to extreme situations for which information in the calibration data set might have been limited. With respect to the control variables, our approach was conservative since we did not optimize the crop rotations themselves, but let the optimization algorithm only chose from a set of crop rotations applicable for the regional conditions.

Genetic algorithms, as all evolutionary approaches, cannot guarantee to find optimal solutions - instead they aim at identifying approximately optimal solutions. Goodness of the results depends most importantly on the algorithm chosen, the population size and the number of evaluations. The NSGA-II algorithm that we used has been successfully applied in the past, but Reed et al. (2013) identified severe search failures for NSGA-II on difficult problems. Since population size has been shown as an especially sensitive parameter for the NSGA-II (Reed et al., 2013), we ran a series of pilot simulations to identify a reliable population size. Based on these simulation results, we selected a population size of 360. Multiple runs with different random seeds led to similar shapes of the Pareto frontier but had a different spread of the solutions. To acknowledge the different spread of the optimization runs, we decided to pool the results and to select those by application of the epsilon dominance. We think that this led to a reliable identification of the Pareto frontier. However, for optimization problems with more than four objectives, or for problems in which sharper changes of the shape of the Pareto frontier have to be expected one should move to next generation genetic algorithms such as Borg (Hadka and Reed, 2012), GDE3 (Kukkonen and Deb, 2006), ε-NSGAII (Kollat and Reed, 2006), AMALGAM (Vrugt and Robinson, 2007), and or the multiple particle swarm optimizer OMOPSO (Sierra and Coello Coello, 2005).

Solution spaces with more dimensions than three are hard to communicate if the different objectives are independent of each other. In addition, our design space is quite complex, since different combinations of crop rotations can be placed in the different HRUs. The data to which the self-organizing map was applied ignored part of the complexity by looking at crop specific yield only while ignoring temporal and spatial effects of crop placement and the effect of the position in the crop rotation. The analysis of the generalized additive models indicated that these effects do play a role in the outcome of the model. Nevertheless, the effects of non-linearity mostly affected high crop yields, and the slopes of the effects were not overly affected by changes of sign. We therefore think that our decision to search for patterns in the data based on the total yields per crop and the water quality and low flow objective can be seen as a reasonable simplification of the problem at hand.

Every unsupervised classification approach, such as self-organizing maps, has to face the problem of a missing goodness of fit criterion that would allow a comparison across different unsupervised classification approaches. However, in our application it was only important to identify useful units for interpretation of groups of management strategies for the watershed. We see those clusters as the hierarchical level to be discussed with stakeholders and decision makers in the first place. If first preferences have been expressed and a limited set of clusters has been identified, further investigation of that limited set of solutions would seem useful. At that stage, solutions from neighboring clusters might be partly included to account for the uncertainty during the clustering step. Further on, aspects of spatial allocation of the crop rotations, the temporal placement of crops and the effect of the crop rotation could also be discussed at this second step.

Future work should investigate different bioenergy crops such as the use of corn for biogas production and investigate the different sources of uncertainty such as model parameterization. In addition, the effect of changing climate conditions on Pareto-optimal solutions should be investigated and robust solutions for different climate scenario assumptions should be sought. Another road to follow would be the use of monetary values such as market prices or contribution margins instead of biophysical yield units. This would shift the perspective from the regional planner towards the farmer. Results would then differ due to changing prices over time, allowing on the one hand a better representation of farmer's livelihood but introducing on the other hand biases due to the heavily subsidized agricultural markets.

While the analysis presented here shows the range of possible options, it cannot show how these options can be reached by policy instruments. To study the effect of policy instruments, one would have to incorporate farmers' behavior, for example by simple agent based models, and use the policy instruments as control variables during the optimization.

## 6 CONCLUSIONS

As an addition to approaches relying on a fixed set of scenarios we identified functional trade-offs of bioenergy production in a medium sized watershed by combining a watershed model with an optimization algorithm. To reduce the search space we looked only for trade-offs with biodiesel crop production based on rapeseed. A reduction of complexity of the results by means of a self-organizing map led to useful units on the four dimensional Pareto-frontier. The derived units seem to be reasonable for communication with stakeholders. Further research should be headed towards the identification of robust solutions under changing environmental conditions and additional biofuel options.

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