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Assessment of nitrogen leaching from arable land in large river basins
Part II: regionalisation using fuzzy rule based modelling

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Abstract

This study deals with fuzzy rule based modelling of nitrogen (N)-leaching from arable land. Main purpose is the elaboration of a method, which allows dynamical regionalisation of results from process-based models for large regions and can be efficiently included in metamodels or decision support systems for rapid integrated assessment of water resources. The paper is the second part of a two-part paper. In the first paper the distributed ecohydrological model SWIM had been applied to calculate and analyse nitrogen dynamics in arable soils for a set of representative natural and management conditions in the Saale River basin (Ecol. Model. (in press)). Here, in the second paper the results from those simulation experiments are used to define, train and validate fuzzy rule systems for the estimation of N-leaching. Nine fuzzy rule systems, specific for nine soil classes, were created from the simulation experiments, representing the conditions for the whole Saale River basin. The fuzzy rule systems operate on monthly time steps and consist of 15 rules and seven input variables each, which are compiled from time series of precipitation, percolation and evapotranspiration as well as from information about fertilizer and crop specific nitrogen uptake. Simulated annealing as a non-linear discrete optimisation method is used for automatic rule assessment. Validation of the fuzzy rule systems, carried out by split sampling of 30-year simulation period, shows satisfactory performance on an annual basis and good performance on the long-term basis with average correlation between SWIM-simulated and fuzzy rule-estimated N-leaching values of 0.78 and 0.94, respectively. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Nitrogen leaching; Dynamic modelling; Large scale; Regionalisation; Fuzzy rules; Simulated annealing

1. Introduction

Diffuse nitrogen (N) emission from agricultural land is one of the major sources of pollution for ground water, rivers and coastal waters. Impact analysis of climate and land use change, assessment of the environmental implications and rec-

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ommendations for sustainable management strategies require adequate mathematical modelling of water and nutrient cycles.

The representation of nitrogen dynamics in models is much more complex compared to the representation of the pure water cycle. It requires the consideration of various physical, biological and chemical processes and their interrelations and can be approximated often only in an integrated modelling approach. Also, the degree of spatial heterogeneity is very high, adding anthropogenic variability of agriculture management to the already high natural variability of climate forcing, soil parameters and state variables. Besides, usually the results of N-modelling are more difficult to validate due to the lack of sufficient measurements.

Over the last two decades several nitrogen dynamics models have been developed. A large number of those models is focussing on the horizontally homogeneous patch scale, dealing mainly with the vertical one-dimensional processes in the unsaturated soil zone (Knisel, 1980; Johnsson et al., 1987; Smith, 1992; Kersebaum, 1995). Further developments have lead to spatially distributed tools for mesoscale basins, which also include approaches for the description of lateral N-fluxes, their retention and decomposition (Young et al., 1989; Arnold et al., 1993; Krysanova et al., 1998). Recently some tools for large scale assessment have been developed, either by extension of former smaller scale process models (Srinivasan et al., 1993) or by model conceptualisations (Arheimer, 1998; Johnes, 1996; Quinn et al., 1996). While the first class of macroscale models has the advantage to use well-tested methods and process-oriented modelling, its disadvantages are high data requirements, uncertainties when using averaged parameters for larger simulation units and time consuming computations. On the other hand, the simplified models have moderate data requirements, are less demanding in modelling effort and have a high potential to become part of integrated models or decision support systems (DSS, Alkemade et al., 1998; Davis et al., 1998). The disadvantage is a certain loss of accuracy and detail.

Purpose of this study is the elaboration of a method for spatially distributed estimation of N-leaching from arable land within large regions, which is suitable to become included into decision support systems for integrated assessment of water and nutrients. This requires not only sufficient accuracy of estimations but also fast and parameter parsimonious calculations. The main idea is to make maximum use of simulation results from process-based models through second order modelling at a generalized level, which is also referred to as metamodel approach (Bouzaher et al., 1993; Bierkens et al., 2000, pp. 105–109; Haberlandt et al., 2001). Considering prospective applications for regional to national environmental management, the primary focus is on reliable simulation of the annual to long-term N-leaching behaviour with an appropriate high spatial resolution between 1 and 10 km.

Following this strategy, a two step procedure is required. In the first step a sufficient large number of simulation experiments with a process-based model have to be carried out. N-leaching at the patch scale is estimated for a representative set of natural (climate, soils, etc.) and management conditions (crop rotations, fertilization) in the region under study. In the second step a regionalisation or upscaling of the results is necessary. There are several alternatives for regionalisation of N-leaching estimates. A straightforward approach is the aggregation and classification of all simulation results into a database (Hoffmann and Johnsson, 1999), which can then be used for planning and assessment of modified land use and management scenarios. Disadvantage of this method is that implications of 'new' inputs (e.g. fertilizer, climate) which are not covered by the range of simulation experiments cannot be evaluated directly. This would require inter- and extrapolation abilities of the regionalisation procedure. For that, conventional statistical models like multiple regression (Børgesen et al., 2001; application to N-loss) or tools of artificial intelligence like regression trees (Dalaka et al., 2000; application to photosynthetic activity), neuronal networks (Nunnari et al., 1998; application to atmospheric pollution data) or fuzzy rule approaches (Bárdossy and Duckstein, 1995; several applications) could be used. Here, any of those methods could be applied on the data sets resulting from the simulation experiments. The conventional regression is easily applied but it requires a quite restricted prescribed model, while the latter methods have more flexible model building capabilities involving often automatic identification procedures.

For this study fuzzy rule based modelling has been chosen as a method for dynamic regionalisation of simulated N-leaching estimates, because of the possible treatment of highly non-linear processes, the transparency of the results (if–then rules) and the ability of the system to include prescribed knowledge as well as the chance for stepwise integration of more results if available. Fuzzy rule based approaches have been successfully utilized for different water resources problems like infiltration modelling (Bárdossy and Disse, 1993), prediction of regional droughts (Pongracz et al., 1999), reservoir operation management (Shrestha et al., 1996) and large scale erosion assessment (Mitra et al., 1998). Once the fuzzy rule system is set up, it can be applied independently from the process-based model for scenario analysis to evaluate different management options or impacts of climate and land use change. Depending on the size and representativeness of the training data set the application is possible for large regions and quite different conditions.

The paper is the second part of a two-part paper. In the first paper the distributed modelling system SWIM (Krysanova et al., 1998) had been applied to calculate and analyse nitrogen dynamics in arable soils for a set of representative natural and management conditions in the Saale River basin (Krysanova and Haberlandt, 2001). Here, in the second paper the results from those simulation experiments are used to define, train and validate fuzzy rule systems for generalized modelling of N-leaching. After the introduction (Section 1) the methodology of the fuzzy rule approach is discussed (Section 2). Study region, input data and the results from simulation experiments with SWIM are briefly described in Section 3. Section 4 is devoted to the application and verification of the fuzzy rule approach for the Saale region and conclusions are drawn in Section 5.

2. Fuzzy rule approach

Basic information about fuzzy set theory can be found in Dubois and Prade (1980) or Zimmermann (1985), and fuzzy rule based modelling is described in Bárdossy and Duckstein (1995). The following focuses on the specific approach, which is used here for the estimation of time series of N-leaching from arable soils. The fuzzy rules are assessed from a training data set and tested using a validation data set; both derived from a limited number of runs with a complex ecohydrological model.

2.1. Fuzzy rules

One fuzzy rule i consists of K arguments in form of fuzzy numbers $A_{i,j}$ with membership functions μ_{Aj} and one response B_i with membership μ_B:

$$\begin{aligned}&\text{IF } (x_1 \text{ is } A_{i,1}) \text{ AND } (x_2 \text{ is } A_{i,2})\\ &\quad \text{AND} \cdots \text{AND} \quad (x_K \text{ is } A_{i,K})\\ &\qquad \text{THEN } (y \text{ is } B_i).\end{aligned} \tag{1}$$

For each input variable x_j ($j = 1, \ldots, K$) and for the output variable y sets of fuzzy numbers $\{A_{j,1}, \ldots, A_{j,N(j)}\}$ and $\{B_1, \ldots, B_{N(y)}\}$, respectively, are predefined. Only triangular fuzzy numbers and 'AND' operators are used here. Fig. 1 illustrates one fictive fuzzy rule with two arguments and one response, selected each from a set of two or three predefined triangular fuzzy numbers.

A fuzzy rule system consist of $i = 1, \ldots, M$ rules and can be represented in the form of a matrix with positive integer values $A_{i,j}$ and B_i.

$$R = \begin{pmatrix} A_{1,1} & \cdots & A_{1,K} & B_1 \\ \vdots & \vdots & \vdots & \vdots \\ A_{M,1} & \cdots & A_{M,K} & B_M \end{pmatrix}. \tag{2}$$

The fuzzy rule system allows, in contrast to ordinary (crisp) rules, partial and simultaneous fulfilment of rules. The overall response of the rule system is a combination of all individual rule responses, taking into account the individual degree of fulfilment of the rules. The fulfilment grade v_i ($0 \le v_i \le 1$) of one fuzzy rule i is assessed using the product inference method:

$$v_i = \prod_{j=1}^{K} \mu_{Ai,\,j}(x_j). \tag{3}$$

In order to simplify the calculations only crisp responses b_i are considered as individual answers for each rule i:

$$b_i = y_l \quad \text{for} \;\; \mu_{Bi}(b_i) = 1.0. \tag{4}$$

Thus, the total answer of the rule system b^* is obtained as sum from the responses of all rules ($i = 1, \ldots, M$) weighed by the fulfilment grades:

$$b^* = \frac{\sum_{i=1}^{M} v_i \cdot b_i}{\sum_{i=1}^{M} v_i}. \tag{5}$$

These calculations are carried out for each time step in the training and validation data sets.

2.2. Assessment of the fuzzy rules

The problem is to find a rule system R with optimal performance $P(R)$. The performance is calculated by comparison of 'observed' values y with simulated responses $y^* = b^*$ for all time steps $t = 1, \ldots, n$ using the sum of mean squared errors as performance function:

$$P = \sum_{t=1}^{n} (y(t) - y^*(t))^2. \tag{6}$$

The number of possible rules is the product of the numbers of fuzzy sets defined for all input variables and the output variable $\Pi_j N_j \times N_y$. This means, that the number of possible rule systems is:

$$\begin{pmatrix} \prod_{j=1}^{K} N_j \times N_y \\ M \end{pmatrix}, \tag{7}$$

which is usually a very large number. For example, in the case of a small rule system with $K = 3$ arguments having $N_j = 6$ possible fuzzy numbers each and the response having $N_y = 7$ possible answers, the number of conceivable rule systems consisting of $M = 5$ rules is:

$$\begin{pmatrix} 6^3 \times 7 \\ 5 \end{pmatrix} \approx 6.5 \times 10^{13}.$$

Thus, it is infeasible to try out all possible rule systems in order to find that one with the optimal performance P. Discrete optimisation provides a way to find a 'good' rule system. Here, simulated annealing (Aarts and Korst, 1989) is applied as optimisation method. The specific procedure is as follows:

1. Definition of possible fuzzy numbers for all arguments $\{A_{j,1}, \ldots, A_{j,N(j)}\}$ and the response $\{B_1, \ldots, B_{N(y)}\}$.
2. Definition of an initial annealing temperature $t_a = t_0$ and a temperature decrease factor dt.
3. Generation of an initial rule system R at random.
4. Calculation of the performance $P(R)$ of the rule system using Eq. (6).
5. Selection of one element of the rule system at random.
6. Allocation of a new possible fuzzy number to the selected element at random.
7. Setting $P_{\text{old}}(R) = P(R)$ and recalculate the performance $P(R)$ using Eq. (6).
8. If $P(R) < P_{\text{old}}(R)$ the change is accepted ('positive changes').
9. If $P(R) \geq P_{\text{old}}(R)$ the change is accepted ('negative changes') with the probability:

$$\pi = \exp\left(\frac{P_{\text{old}}(R) - P(R)}{t_a}\right).$$

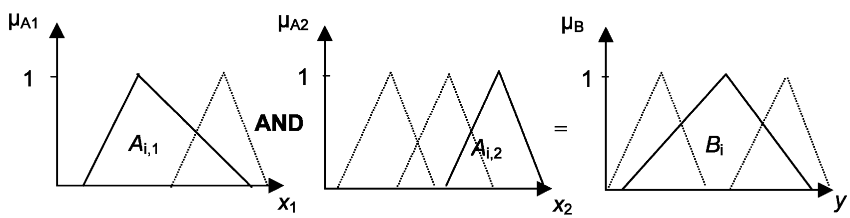

Fig. 1. Scheme of one fictive fuzzy-rule.

10. Steps 5–9 are repeated m times.
11. The annealing temperature t_a is reduced: $t_{a+1} = dt \times t_a$ with $0 < dt < 1$.
12. Steps 10 and 11 are repeated until the number of positive changes becomes smaller than a threshold ip_{stop}.

The above algorithm yields a rule system with 'optimal' performance. Step 9 ensures, that the optimisation does not stop at any local minima but will converge toward a global minima. The annealing temperature t_a regulates the probability of negative changes. The lower t_a the less likely the acceptance of a negative change. The convergence is ensured in reducing the temperature each time after m iteration steps. The procedure allows the inclusion of predefined or partly predefined rules by fixing certain elements of R, which will be excluded in the selection step 5. Additional information about parameters and constraints of the procedure are given together with the description of the application in Section 4.

3. Simulation experiments

The first step of the proposed regionalisation procedure involves the selection of a suitable model for process-based simulations of nitrogen dynamics and the application of that model for a representative set of variants (simulation experiments) in a macro-scale study region. The selected model, the study basin, the definition and evaluation of the simulation experiments have been discussed in greater detail in the first paper (Krysanova and Haberlandt, 2001). Here, only a summary is given, focussing on the simulation experiments.

The distributed SWIM modelling system (Krysanova et al., 1998) has been chosen as a simulation tool. SWIM includes as its kernel a continuous-time spatially distributed model, integrating hydrology, crop-vegetation, nutrients (nitrogen, N and phosphorus, P) and sediment transport at the river basin scale. All processes are simulated at a daily time step. For this study only the nitrogen dynamics at a horizontally homogeneous quasi point scale are considered. Although, a point model would be sufficient here, the advantage of SWIM is the possibility for a validation at the river basin scale using observed discharge and nitrogen loads. Several studies have shown the ability of SWIM to simulate hydrology and nitrogen dynamics in a satisfactory manner at the basin scale level (Krysanova and Becker, 1999; Krysanova et al., 1999). For this study the results of a hydrological validation are shown in the first paper (Krysanova and Haberlandt, 2001).

The capability of the fuzzy rule approach to simulate N-leaching for a wide range of prospective scenarios depends on an appropriately chosen and representative training data set. Simulation experiments were planned according to the occurring variation in natural and management conditions for agricultural areas in the 23 687 km^2 Saale River basin, a large sub-basin of the Elbe, with agricultural land occupying about 63% of the drainage area. Fig. 2 shows the location, the main rivers and the topography of the Saale River basin with the reference climate stations indicated (see below).

To make the procedure straightforward, only a subset with the most relevant variants described in the first paper (Krysanova and Haberlandt, 2001) is used here. Four of five reference climate stations are chosen considering simultaneously long-term average annual precipitation and average temperature. One high-elevation station, whose climate is only applicable for about 1% of the arable land has been excluded. Besides, higher elevation classes are neglected here, given that the focus is on total N-losses with water not differentiating between flow components (surface runoff, interflow and percolation to groundwater). Soils occurring on arable land (Hartwich et al., 1995) were classified into nine classes taking into account the soil field capacity and saturated hydraulic conductivity as well as the occurrence of soils in agriculture land. Three crop rotations and three fertilization schemes were created in accordance with usual practices in the area (Roth et al., 1998; Krönert et al., 1999) and by assuming simple intensification and extensification scenarios. Table 1 summarizes the selected variants, resulting in 324 cases (four climates × nine soil classes × three crop rotations × three fertiliza-

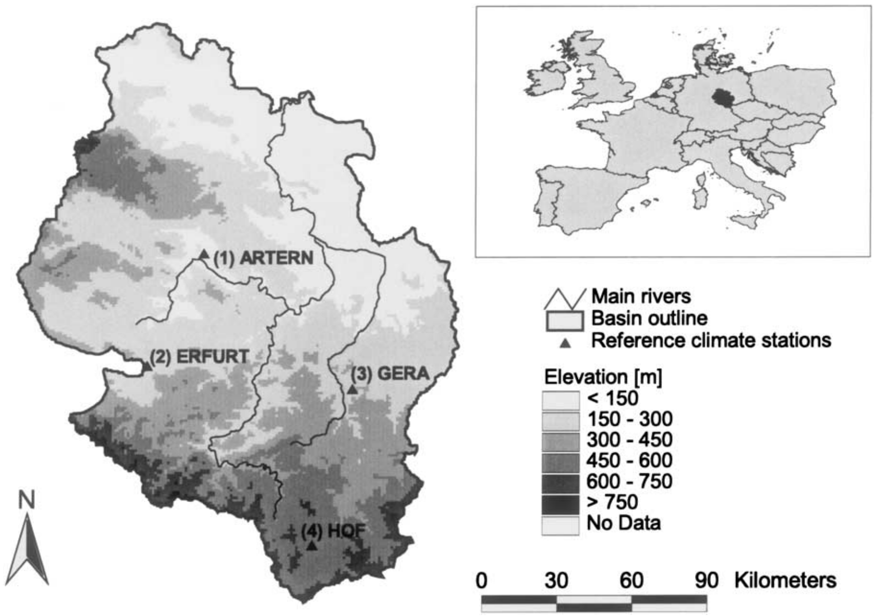

Fig. 2. Location, main rivers and topography of the Saale River Basin with reference climate stations indicated.

Table 1
Overview of the simulation variants

Factor	Classification
Soil profile	Nine soil classes comprising each between one and five profiles according to the German soil map BÜK1000 (Hartwich et al., 1995): 1 = s09, 2 = s36, 3 = s51, 4 = s59, 5 = s40, 6 = s56, 7 = s38, 8 = s43, 9 = s55
Climate region	Four climate regions classified according to average precipitation and temperature using four climate stations (30-year period: 1961-90): c1 = Artern, c2 = Erfurt, c3 = Gera-Leumnitz, c4 = Hof-Hohensaas
Crop rotation	Three crop rotation schemes, each 10 years in length: (r1) basic: pot, ww, sb, wr, grass, ww, wb, pot, ww, ma; (r2) intensive: pot, wb, ma, ww, wr, ww, ma, pot, ww, ma; (r3) extensive: pot, grass, sb, wr, grass, ww, wb, pot, ww, grass
Fertilization	Three fertilization schemes: (f1) standard: on average 166 kg/ha inorganic + 60 kg/ha organic; (f2) + 50%: on average 249 kg/ha inorganic + 90 kg/ha organic; (f3) − 50%: on average 83 kg/ha inorganic + 30 kg/ha organic

For details see Krysanova and Haberlandt (2001). ww, winter wheat; wb, winter barley; wr, winter rye; sb, summer barley; pot, potato; ma, silage maize.

tions). SWIM was applied to each variant for the 30-year period from 1961 to 1990 on a daily time step.

The results of the simulation runs are analysed in detail in the first paper (Krysanova and Haberlandt, 2001). A comprehensive assessment of the sensitivity of the modelled N leaching to variations in natural and anthropogenic conditions led to the conclusion, that the relative importance of the influencing factors decreases as follows: (1) soil; (2) climate; (3) fertilization rate; and (4) crop rotation.

4. Application

This section describes the application of the fuzzy rule approach for the Saale River basin including the pre-processing of the results from the simulation experiments, the identification of the fuzzy rule system and the validation of the approach.

4.1. Data pre-processing

One of the most important steps for the identification of a fuzzy rule system is the selection and compilation of the input variables. They should have significant impact on the nitrogen dynamics and be easily available for future scenario analysis without the need for running a process-based model. Although the primary focus is on a good simulation of the annual to long-term behaviour of N-losses, a monthly time step has been chosen for the fuzzy rule approach. This allows to consider important seasonal climate and management effects and is a compromise between the high non-linear process dynamics and the required computational efficiency of the solution. Table 2 lists some important variables, which are evaluated amongst several others regarding their use for the fuzzy model. The list mainly comprises routinely observed climate variables, simulated water fluxes from a conceptual hydrological model, fertilization amounts and specific values of average crop uptake of N.

Precipitation (PCP) and air temperature (TAV) are observed variables at the climate stations. Water outflow (Q) is the sum over three flow components leaving the soil column (surface runoff + interflow + percolation to ground water). Both Q and evapotranspiration (ETR) are simulated by SWIM. Fertilization amounts (FERT) comprise mineral and organic N components, with the latter transformed by a constant factor of 0.42 into inorganic equivalents. This factor has been estimated from simulations with SWIM comparing average N-mineralization amounts for different organic N quantities applied. Atmospheric N deposition is modelled in SWIM proportional to the precipitation amount and therefore can be neglected here for the test of the fuzzy rule systems (i.e. it is sufficiently explained by PCP and Q). Crop uptake of N ($NUPT_{12}$) can

Table 2
Important variables used for the identification and application of the fuzzy model

No.	Symbol	Variable	Units	Source for identification	Source for application
1	PCP	Monthly precipitation sum	mm per month	Clistat	Clistat
2	TAV	Average monthly air temperature	°C	Clistat	Clistat
3	Q	Total water outflow current month	mm per month	SWIM	Hymod
4	Q_{-1}	Total water outflow last month	mm per month	SWIM	Hymod
5	Q_{12}	Average water outflow over last 12 months (excluding current month)	mm per month	SWIM	Hymod
6	Q_{sald}	Difference between total PCP and total Q over the whole simulation period for each variant	mm per year	SWIM	Hymod
7	ETR	Evapotranspiration	mm per month	SWIM	Hymod
8	FERT	Fertilization current month	kg N/ha per month	Variant	Scenario
9	$FERT_{12}$	Average monthly fertilization over last 12 months (including current month)	kg N/ha per month	Variant	Scenario
10	$NUPT_{12}$	Specific nitrogen crop uptake averaged over the last 12 months (including current month)	kg N/ha per month	Parameter (SWIM)	Parameter (SWIM)
11	$FERT_{sald}$	Difference between total FERT and total NUPT over the whole simulation period for each variant	kg N per year	Variant + parameter	Scenario + parameter
12	N_{out}	N-leaching (target variable)	kg N/ha per month	SWIM	(output)

Clistat, observations from climate stations; hymod, simple vertical water balance model; parameter, quasi constant values; variant, defined for simulation experiments; scenario, defined for impact analysis.

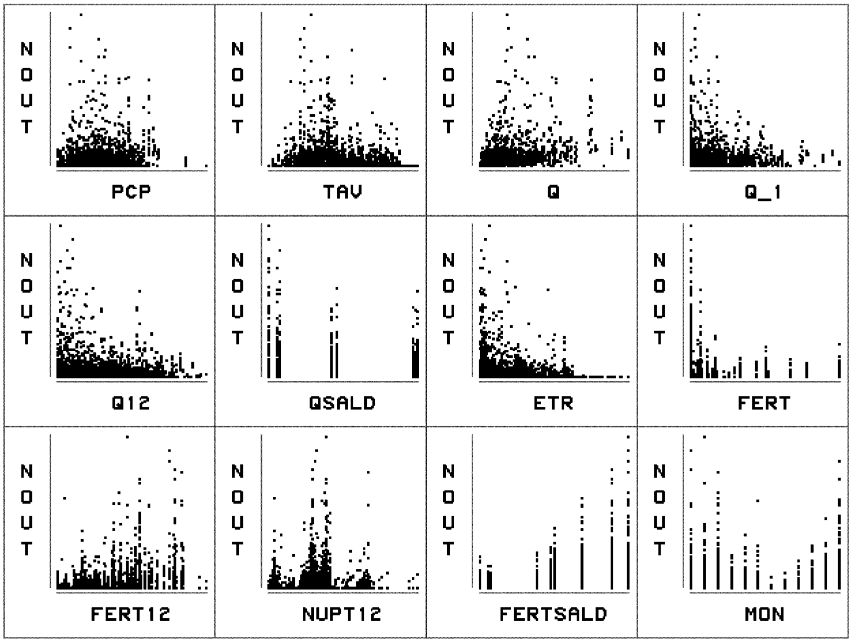

Fig. 3. Relation between monthly N-leaching (N_{out}) and several prospective input variables for the fuzzy model for the soil class s56 (training period: 1961–1970 and 1981–1990).

be considered as averaged fixed plant specific parameters (from 12 values per crop, one for each month), which is assessed from long-term SWIM simulations and can also be used for future applications. To consider a certain hydrological memory in the fuzzy rule systems, several lagged and aggregated variables are introduced: water outflow from the previous month (Q_{-1}), water outflow over the last 12 months (Q_{12}) and average fertilization over the last 12 months ($FERT_{12}$). The finally selected levels of aggregation and lags are based on experience and some initial tests. Besides, some total balances (Q_{sald} and $FERT_{sald}$) are used to distinguish between general 'site' conditions represented by each of the variants (36 variants per soil class: combination of climates, fertilizations and crop rotations). All dynamic process variables describing the nitrogen cycle, like N content in soil, denitrification, mineralization etc. have been avoided. However, hydrological fluxes like water outflow and evapotranspiration are included, assuming they can be obtained in a future operational case from a simple conceptual vertical water balance model. N-leaching (N_{out}) is the target variable to be modelled. It is considered to be the sum of three nitrogen flow components leaving the soil profile with water (N-wash-off with surface runoff and interflow and N-leaching to groundwater).

As an initial assessment about the value of the input variables, a correlation analysis is carried out. Fig. 3 shows simplified scatterplots between monthly N-leaching and several explanatory variables. It becomes obvious, that the relationship between N-leaching and the input variables is non-linear and that there is no single variable with a dominating effect on N_{out}. Actual N-leaching increases with increasing Q, $FERT_{12}$, $FERT_{sald}$ and with decreasing Q_{-1}, Q_{12}, ETR. Note, that actual N-leaching seems not to originate mainly from current fertilization (FERT), but rather than from past applications ($FERT_{12}$). Regarding $NUPT_{12}$, PCP and TAV the potential for leaching is highest for values in the middle of the input range. A comparison for different months shows higher leaching values during the winter season.

Further analysis is required to decide about an optimal number and combination of input variables (see Section 4.2).

4.2. Model identification

The building of the fuzzy model involves basically the following three tasks, which are discussed in this section:

(a) the definition of the structure of the model (variables, number of systems and rules);
(b) the definition of fuzzy numbers on input variables and on the response; and
(c) the assessment of the fuzzy rules (optimisation of the arguments for the rules).

Steps (b) and (c) are done by automatic procedures. For step (a) quite a bit of manual testing and sensitivity analysis has been carried out here, also to gain experience and reduce the pre-processing work for future similar cases.

To guarantee a maximal flexibility of the fuzzy model for possible future scenario analysis, it would be optimal to identify a single fuzzy rule system based on the combined data from all of the 324 variants. However, this would require a sufficient parameterization of the soil types addressing their N-leaching behaviour, which has failed so far in preliminary tests. So, in the approach taken here nine separate fuzzy rule systems are defined according to the nine soil classes, each based on data from all combinations of climates, crop rotations and fertilization (36 variants). This significantly improves the simulation quality compared to a single rule system for all soils, since soil types have the strongest impact on N-leaching among all factors considered (see Krysanova and Haberlandt, 2001). However, this strategy implies some concession to the flexibility of the approach.

For the whole identification process the data set is divided into two samples, one for training and one for validation. This is done by splitting the 30-year simulation period (1961–1990) into 20 years for training (1961–1970 and 1981–1990) and 10 years for validation (1971–1980). The validation set is taken from the middle part of the whole period to avoid inconsistencies between the learning and training sets caused by trends. So, altogether each data set for training and validation consists of 8640 and 4320 records of monthly data, respectively (one soil $\times$ four climates $\times$ three crop rotations $\times$ three fertilization schemes $\times$ 20/10 years $\times$ 12 months).

A decision about the number of variables and the number of rules has to be made before the assessment of the rule systems (see also Section 2). In addition to the information gained from the correlation analysis, further trial and error testing is carried out here. Several fuzzy rule systems with different number and combination of input variables are assessed. Fig. 4 shows some of the results for three selected soil classes using rule systems with 15 rules each. Comparing the standard errors, conclusions about the relevance of the number and selection of specific variables can be drawn. First, it can be seen that using percolation (Q) and evapotranspiration (ETR) instead of precipitation (PCP) and air temperature (TAV) decreases the errors significantly. Adding actual fertilization (FERT) as input variable does not improve the results, but using the average fertilization over the last 12 months ($FERT_{12}$) does. Further improvements are made by inclusion of the average outflow over the last 12 months (Q_{12}). The specific plant uptake over the last 12 months ($NUPT_{12}$) as a single variable has no effect, but utilized as a component in the fertilization saldo ($FERT_{sald}$) it seems quite useful. Also, the incorporation of the flow saldo (Q_{sald}) is helpful. Generally, the differences between the various combinations of variables are more pronounced as higher the leaching potential of the soil is (see Section 3). Concluding from those experiments, seven input variables have been chosen for all nine fuzzy rule systems: Q, Q_{-1}, ETR, $FERT_{12}$, Q_{12}, $FERT_{sald}$ and Q_{sald}.

Regarding the optimal number of rules similar tests are run. In this case the problem of ‘overfitting’ can be serious. Fig. 5 shows this effect by comparing standard errors in relation to the number of rules averaged for three selected soil classes for the training and the validation period. While with increasing number of rules the performance for the training period becomes continually better, the performance for the validation period does not follow this pattern. The latter even decreases

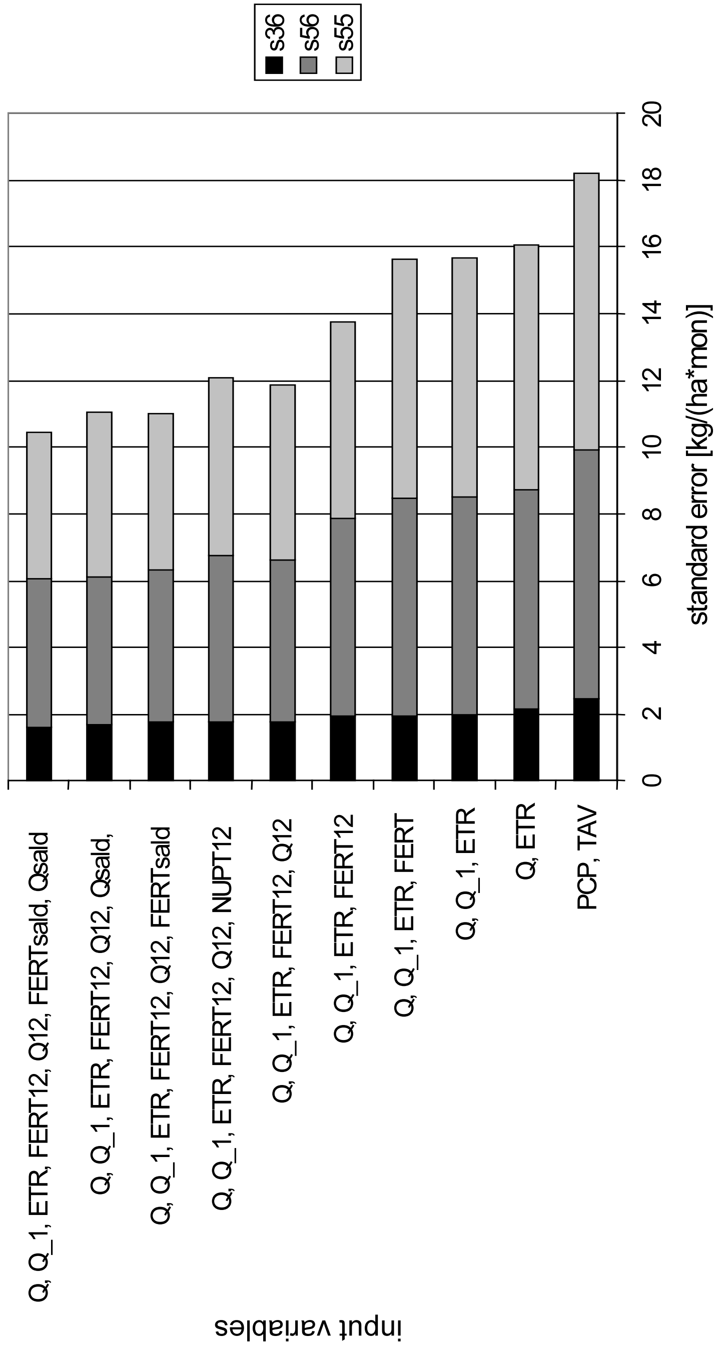

Fig. 4. Cumulative performance of the fuzzy rulea systems for three selected soil classes: s36, s56, s55 using different numbers and combination of input variables (training period: 1961–1970 and 1981–1990).

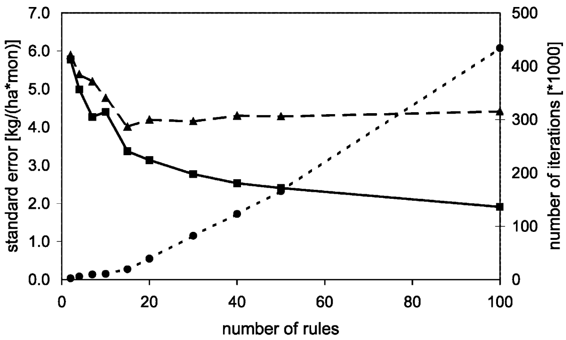

Fig. 5. Performance for training (solid line) and validation (dashed line) periods and required total number of iterations until ip_{stop} is reached (dotted line) for fuzzy rule systems using different number of rules, averaged for three selected soil classes: s36, s56 and s55.

again with higher number of rules (> 20). For a robust approach the simulation results for both training and validation periods should show low errors in a similar range. This is the case for a moderate number of rules in the middle between 10 and 20. So, for subsequent modelling the number of rules is set arbitrarily to 15 for all nine rule systems. Fig. 5 also shows the total number of required iterations to reach the stop criterion (ip_{stop}, see Section 2) in relation to the number of rules in the system. It can be seen that the number of iterations can become quite large, which increases the learning time dramatically.

Another important issue is the adequate definition of fuzzy numbers on the input variables and on the response. After some tests an automatic procedure is used considering the range of the variables and the frequency of the values. As mentioned before, only triangular fuzzy numbers are employed. Fig. 6 shows exemplarily the fuzzy numbers defined on the input variable 'average fertilization over the last 12 months' ($FERT_{12}$). Given any total number N of fuzzy numbers to be defined on one variable, the procedure associates one fuzzy number for the infinite case (e.g. grey line parallel to x-axis in Fig. 6), one for the zero case (e.g. vertical grey line by $x_i = 0$ in Fig. 6), three symmetric numbers equally partitioning the observed range of the variable (e.g. three triangles with black lines in Fig. 6) and the remaining $(N-5)$ according to the frequency of the values (e.g. three triangles with dashed lines in Fig. 6) with the largest fuzzy number extending to infinity of x. From experience N is set here to values between 6 and 12, with 12 for the response variable and decreasing number according to the relevance of the input variables. Finally, the fuzzy numbers are ordered by maximum (i.e. by the value of x_i for $\mu(x_i) = 1$), the Euclidian distance

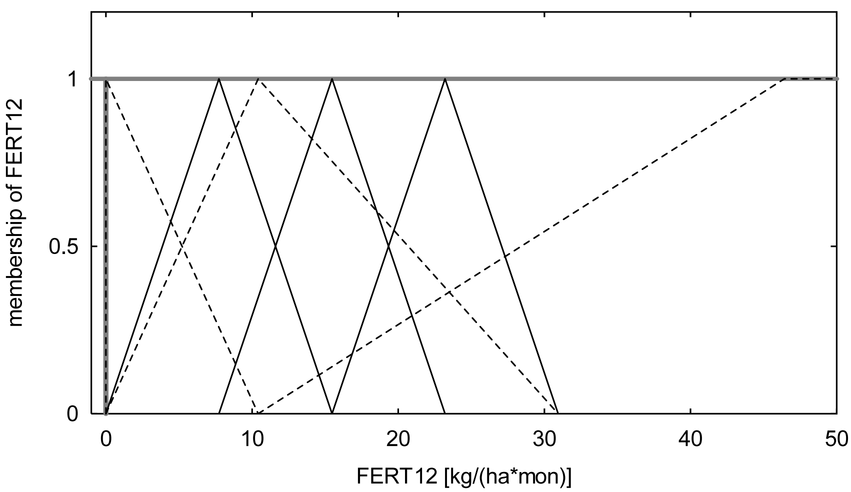

Fig. 6. Fuzzy numbers defined on the input variable 'average fertilization over the last 12 months' ($FERT_{12}$); horizontal and vertical solid grey lines: infinite and zero cases, respectively; solid black triangles: equal range partitioning; dashed triangles: frequency partitioning.

between adjacent numbers is calculated (see Bárdossy and Duckstein, 1995, p. 31) and for very similar numbers only one is kept. In order to account for values outside the range for future applications the smallest and the largest fuzzy numbers are shifted by 50% beyond the minimum and the maximum values observed, respectively. Fuzzification, ordering, distance calculation and final selection of fuzzy numbers are done automatically. Only the number of fuzzy numbers for each variable has to be set manually.

For the assessment of the fuzzy rules simulated annealing is used as an automatic procedure (see also Section 2), but with the possibility to include some rules a priori. Here only one fixed rule is prescribed: "If percolation is zero than N-leaching is zero, too". This rule is implemented as an exclusive crisp rule disabling the remaining fuzzy rules, since simultaneous fulfilment is undesirable in this case. As objective function P the sum of mean squared errors between SWIM simulated ('observed') and fuzzy rule simulated monthly N-leaching values is taken (see Eq. (6)). The iteration is stopped if the sum of positive changes (i.e. steps where the objective function value decreases) remains smaller than $ip_{stop} = 3$ during the last three temperature loops. Additionally, a parameter v_{lim} is introduced, which leads to a penalty on the objective function value if the sum of the degree of fulfilment over all time steps for a certain rule becomes smaller then v_{lim}. This forces the optimisation procedure to general applicable rules and prevents too strong emphasis on very rare events. With a value of $m = 200$ iterations per temperature loop, a temperature decreasing factor of $dt = 0.98$ and a parameter of $v_{lim} = 10$, the optimisation procedure required a total of about 50 000 steps on average to reach the optimum for each of the nine fuzzy rule systems.

4.3. Results and validation

The nine soil-specific fuzzy rule systems consisting of 15 rules and seven input variables each are assessed and validated considering the above defined prerequisites and data sets for training and validation. Table 3 shows performance criteria for the fuzzy model, listed separately for the training and validation periods as well as for different time scales. The performance improves with increasing time scale. The results are satisfactory for annual values and quite good for long-term ones, which is the most important scale for potential future use of the method. The simulation quality for the training period is better than for the validation period, but the differences are moderate, which demonstrates the robustness of the approach.

In Fig. 7 the annual time series simulated by SWIM and by the fuzzy model for the validation period for the soil class s56 are shown. Considering the graphical representation and the statistical performance criteria (bias = -0.84 kg/ha per year, relative standard error = 0.76, correlation = 0.75) the overall performance is acceptable. However, the extreme values are not modelled very well by the fuzzy rule approach, i.e. an overestimation of minima for climates 3 and 4 and an underestimation of maxima for climates 2, 3 and 4 occurs. This phenomena is typical for the optimisation of models, which use as objective function the standard error and leads generally to a loss of variance. Tests with other performance functions addressing more the extremes (e.g. sum of differences raised to the power of 2.5 or 3.0 instead of 2) showed somewhat better variance reproduction but increased mean errors. Considering the main goal of a good representation of the long-term average N-losses, smaller mean errors are more important than a very good reproduction of the variance or the extremes for single years.

To assess the differences between a conventional linear and a non-linear approach the fuzzy rule approach is compared with a multiple linear regression model. As an example the soil profile s56 is chosen here, too. The same seven input variables as utilized in the fuzzy model are used here as independent variables in the multiple regression approach. Also, all records with zero N-losses are excluded to account for the crisp rule: "If percolation is zero than N-leaching is zero, too". The multiple regression model is fitted for the training period and then applied for the validation period using the monthly data. One problem is the occurrence of negative values for some of the responses. This could have been

Table 3
Performance of the fuzzy rule systems for all nine soil classes

Soil class	Average N-loss (kg/ha per year)	Monthly			Annual		Long-term	
		Bias (kg/ha per month)	SE/average	r	SE/average	r	SE/average	r
Training (1961–1970 and 1981–1990)								
s09	1.8	0.00	1.60	0.85	0.56	0.93	0.09	1.00
s36	9.2	−0.02	2.20	0.80	0.74	0.86	0.19	0.97
s51	11.2	0.01	1.51	0.69	0.49	0.76	0.14	0.93
s59	15.0	0.01	1.40	0.84	0.49	0.87	0.13	0.97
s40	22.2	0.02	2.15	0.85	0.72	0.89	0.15	0.98
s56	30.1	0.01	1.78	0.84	0.61	0.88	0.18	0.97
s38	31.7	0.12	2.21	0.86	0.75	0.89	0.18	0.98
s43	37.90	0.16	1.59	0.86	0.57	0.90	0.22	0.95
s55	42.9	−0.09	1.33	0.86	0.49	0.91	0.16	0.97
Validation (1971–1980)								
s09	2.1	−0.02	2.41	0.75	0.84	0.85	0.34	0.96
s36	7.2	0.25	2.67	0.78	1.04	0.82	0.58	0.97
s51	11.5	−0.11	1.42	0.61	0.60	0.67	0.26	0.91
s59	16.1	−0.18	2.01	0.64	0.70	0.66	0.27	0.89
s40	19.9	0.14	2.21	0.77	0.69	0.86	0.23	0.97
s56	30.5	−0.07	2.15	0.70	0.76	0.75	0.29	0.91
s38	32.4	−0.21	2.36	0.75	0.76	0.83	0.21	0.97
s43	42.4	−0.19	1.73	0.80	0.62	0.81	0.22	0.95
s55	49.4	−0.79	1.60	0.81	0.64	0.79	0.32	0.94

SE, standard error; r, correlation.

avoided by a suitable variable transformation. However, for simplicity and to keep a pure linear approach the remaining small number of negative responses after aggregation to annual values (2% negative values left) has been set to zero. Fig. 8 shows the aggregated annual time series simulated by SWIM and by the regression model. Considering the weak correspondence of the graphs and the high bias and standard error (bias = 17.33 kg/ha per year, relative standard error = 1.04, correlation = 0.75), it becomes obvious that the multiple regression approach is worse compared to the fuzzy model. This is mainly due to the fixed linear regression model, which cannot account for different behaviour of different cases and tries to find average parameters (see Fig. 8 underestimation for dryer climates: period 1–180 and overestimation for wetter climates: period 181–360). In addition, the high bias for the validation period (which is per definition zero for the training period) indicates poor robustness of this approach. Although it is certainly possible to construct better and quasi non-linear regression models by special transformations on the variables, it would be difficult to achieve the performance of the more flexible fuzzy model, which is not forced a priori to any internal model structure. Similar results have been reported e.g. by comparison of neuro-fuzzy networks with autoregressive models for modelling of atmospheric pollution (Nunnari et al., 1998) or by comparison of regression tree modelling with traditional regression for modelling of photosynthetic activity (Dalaka et al., 2000).

Fig. 9 compares in scatterplots the SWIM and the fuzzy rule based simulations of the long-term average N-losses for three selected soil classes and for both training and validation periods. This figure supports the former conclusion about good long-term performance of the fuzzy model. However, it also shows, stressed by the regression lines, that there is a slight systematic error for the validation periods (s36: overestimation, s55: underestimation). For large-scale assessment also the spatial distribution of N-losses for the whole region is important. Fig. 10 shows maps with spa-

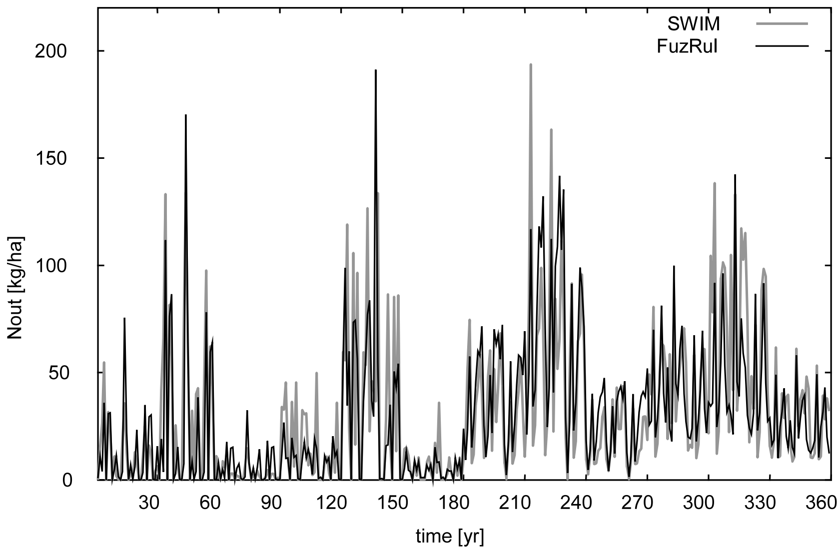

Fig. 7. Annual N-loss time series for soil class s56 simulated by SWIM and by the fuzzy model (FuzRul) for the validation period (1971–1980). The figure shows sequences of 36 × 10 years simulations comprising all variants with crop rotations (r1 … r3) cycling fastest, then fertilizations (f1 … f3) and finally 'climates' (c1 … c4) from left to right (e.g. r1f1c1, r2f1c1, r3f1c1 for the first 30 years etc.).

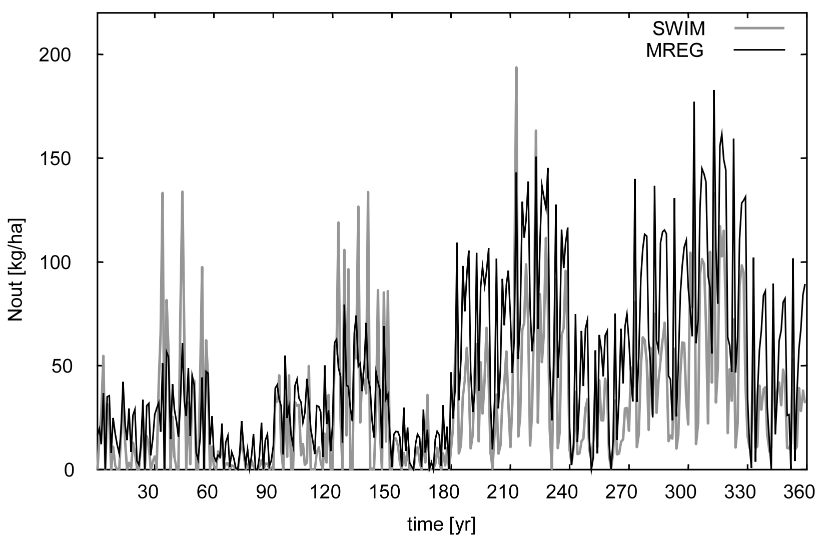

Fig. 8. Annual N-loss time series for soil class s56 simulated by SWIM and by the multiple regression model (MREG) for the validation period (1971–1980). The figure shows a sequences of 36 × 10 years simulations comprising all variants with crop rotations (r1 … r3) cycling fastest, then fertilizations (f1 … f3) and finally 'climates' (c1 … c4) from left to right (e.g. r1f1c1, r2f1c1, r3f1c1 for the first 30 years etc.).

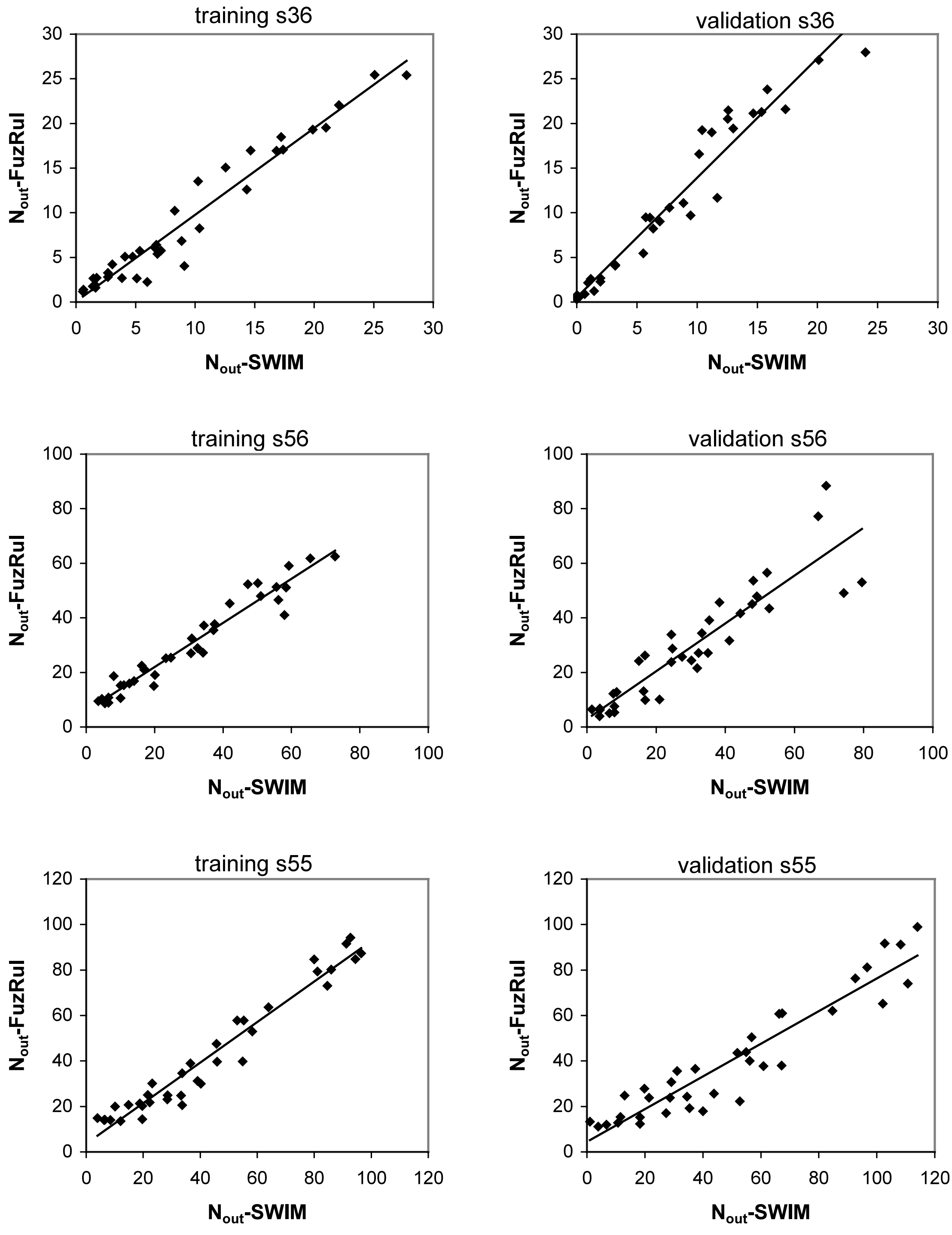

Fig. 9. Long-term N-losses simulated by SWIM and by the fuzzy model for three selected soil classes and both training and validation periods (36 variants per graph: four climates × three rotations × three fertilizations; units: kg/ha per year; correlation see Table 3).

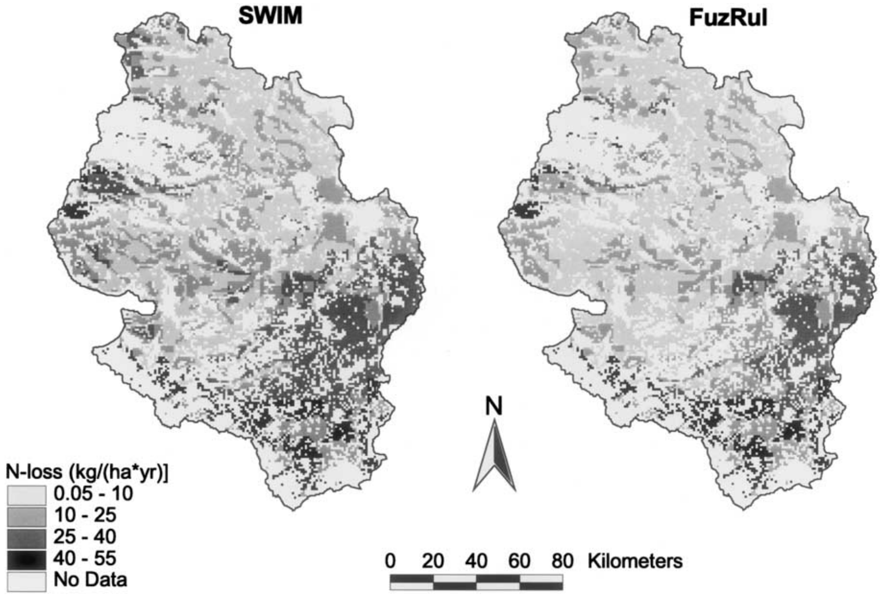

Fig. 10. Spatial pattern of SWIM- and fuzzy-rule simulated N-loss from agricultural soils for rotation 1 and fertilization 1 in the Saale River Basin (total period: 1961–1990).

tially distributed N-losses for arable land within the whole Saale River basin over the total simulation period (1961–1990). The differences between SWIM simulated and fuzzy rule based patterns are very small.

5. Conclusions

The paper has been dealing with fuzzy rule based modelling of N-losses from arable land. Main purpose of this study was the elaboration of a method for spatially distributed estimation of N-leaching within large regions, which is suitable to become included into decision support systems for integrated assessment of water and nutrients. The fuzzy rules are defined and calibrated using results from simulation experiments carried out with the deterministic SWIM modelling system. The fuzzy model has been tested successfully for agricultural areas in the 23 687 km^2 Saale River basin, a large sub-basin of the Elbe. The following points summarize the main results:

1. Fuzzy rule based modelling provides a fast, transparent and parameter parsimonious way for simplified modelling of N-leaching.
2. The approach is especially suitable for generalisation and regionalisation of results from deterministic models.
3. The model performance is good for the estimation of long-term average N-losses, which is the most important time scale for policy exercises.
4. Expert knowledge can be included via a priori fixed rules in the system.
5. Robustness and transferability can be ensured by limiting the number of rules and the number of cases a rule is applied.
6. The assessment of the fuzzy rules can be realized quite easily using simulated annealing as a discrete optimisation method.

Although the results are obtained for a quite restricted and simplified number of management condition in the Saale River basin, it is assumed, that the method can be applied for a wider range and more complex situations as well as for other regions with similar success. For independent applications the method requires external forcing by time series of percolation and evapotranspiration, which can be obtained from a simple conceptual vertical water balance model. Special aspects which are intended to be addressed in the future include the development of a suitable parameterization of the soils in order to merge the soil–class-specific systems into one general fuzzy rule system, the integration of results from more than one deterministic model to reduce model specific bias, extended testing of the system for other regions and applications of the system for scenario analysis.

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References

Aarts, E., Korst, J., 1989. Simulated Annealing and Boltzmann Machines. John Wiley & Sons, New York, NY.

Alkemade, J.R.M., van Grinsven, J.J.M., Wiertz, J., Kros, J., 1998. Towards integrated national modelling with particular reference to the environmental effects of nutrients. Environ. Pollution 102 (Suppl. 1), 101–105.

Arheimer, B., 1998. Riverine nitrogen—analysis and modelling under Nordic conditions. PhD thesis, Linköping University, Sweden, 64 p.

Arnold, J.G., Allen, P.M., Bernhardt, G., 1993. A comprehensive surface-groundwater flow model. J. Hydrol. 142, 47–69.

Bárdossy, A., Disse, M., 1993. Fuzzy rule-based models for infiltration. Water Resour. Res. 29 (2), 373–382.

Bárdossy, A., Duckstein, L., 1995. Fuzzy Rule-Based Modelling with Applications to Geophysical, Biological and Engineering Systems. CRC Press, Boca Raton, FL, p. 232.

Bierkens, M.F.P., Finke, P.A., de Willigen, P., 2000. Upscaling and Downscaling Methods for Environmental Research. Developments in Plant and Soil Sciences, vol. 88. Kluwer Academics Publishers, Dordrecht, p. 90.

Børgesen, C.D., Djurhuus, J., Kyllingsbæk, A., 2001. Estimating the effect of legislation on nitrogen leaching by upscaling field simulations. Ecol. Model. 136 (1), 31–48.

Bouzaher, A., Lakshminarayan, P.G., Cabe, R., Carriquiry, A., Gassman, P.W., Shogren, J.F., 1993. Metamodels and nonpoint pollution policy in agriculture. Water Resour. Res. 29, 1579–1587.

Dalaka, A., Kompare, B., Robnik-Šikonja, M., Sgardelis, S.P., 2000. Modelling the effects of environmental conditions on apparent photosynthesis of Stipa bromoides by machine learning tools. Ecol. Model. 129 (2–3), 245–257.

Davis, J.R., Farley, T.F.N., Young, W.J., Cuddy, S.M., 1998. The experience of using a decision support system for nutrient management in Australia. Wat. Sci. Tech. 37 (3), 209–216.

Dubois, D., Prade, H., 1980. Fuzzy Sets and Systems: Theory and Applications. Academic Press, New York, p. 393.

Haberlandt, U., Krysanova, V., Klöcking, B., Bárdossy, A., 2001. Development of a metamodel for large-scale assessment of water and nutrient fluxes—first components and initial tests for the Elbe River basin. IAHS Publ. no. 268, pp. 263–269.

Hartwich, R., Behrens, J., Eckelmann, W., Haase, G., Richter, A., Roeschmann, G., Schmidt, R., 1995. Bodenübersichtskarte der Bundesrepublik Deutschland 1: 1000000 (BÜK1000). Karte mit Erläuterungen, Textlegende und Leitprofilen. Bundesanstalt für Geowissenschaften und Rohstoffe, Hannover.

Hoffmann, M., Johnsson, H., 1999. A method for assessing generalised nitrogen leaching estimates for agricultural land. Environ. Model. Assess. 4, 35–44.

Johnes, P.J., 1996. Evaluation and management of impact of land use change on the nitrogen and phosphorus load delivered to surface waters: the export coefficient modelling approach. J. Hydrol. 183, 323–349.

Johnsson, H., Bergström, L., Jansson, P.E., Paustian, K., 1987. Simulated nitrogen dynamics and losses in a layered agricultural soil. Agric. Ecosyst. Environ. 18, 333–356.

Kersebaum, K.C., 1995. Application of a simple management model to simulate water and nitrogen dynamics. Ecol. Model. 81 (1–3), 145–156.

Knisel, W.G. (Ed.), 1980. CREAMS: A field scale model for chemicals, runoff, and erosion from agricultural management systems, vol. 26. USDA Conservation Research Report, 643 pp.

Krönert, R., Franko, U., Haferkorn, U., Hülsbergen, K.-J., Abraham, J., Biermann, S., Hirt, U., Mellenthin, U., Ramsbeck-Ullmann, M., Steinhardt, U., 1999. Gebietswasserhaushalt und Stoffhaushalt in der Lößregion des Elbegebietes als Grundlage für die Durchsetzung einer nachhaltigen Landnutzung, Scientific Report. UFZ Leipzig-Halle GmbH, Leipzig, Germany.

Krysanova, V., Becker, A., 1999. Integrated modelling of hydrological processes and nutrient dynamics at the river basins scale. Hydrobiologia 410, 131–138.

Krysanova, V., Haberlandt, U., 2001. Assessment of nitrogen leaching from arable land in large river basins. Part I: simulation experiments using a dynamic model. Ecol. Model. 150 (3), 255–275.

Krysanova, V., Gerten, D., Klöcking, B., Becker, A., 1999. Factors affecting nitrogen export from diffuse sources: a modelling study in the Elbe basin. In: L. Heathwaite (ed.), Impact of Land-Use Change on Nutrient Loads from Diffuse Sources. IAHS Publ. no. 257, pp. 201–212.

Krysanova, V., Müller-Wohlfeil, D.-I., Becker, A., 1998. Development and test of a spatially distributed hydrological/water quality model for mesoscale watersheds. Ecol. Model. 106 (1–2), 261–289.

Mitra, B., Scott, H.D., Dixon, J.C., McKimmey, J.M., 1998. Applications of fuzzy logic to the prediction of soil erosion in a large watershed. Geoderma 86 (3–4), 183–209.

Nunnari, G., Nucifora, A.F.M., Randieri, C., 1998. The application of neural techniques to the modelling of time-series of atmospheric pollution data. Ecol. Model. 111 (2–3), 187–205.

Pongracz, R., Bogardi, I., Duckstein, L., 1999. Application of fuzzy rule-based modeling technique to regional drought. J. Hydrol. 224, 100–114.

Quinn, P., Anthony, S., Lord, E., Turner, S., 1996. Nitrate modelling for the UK: a Minimum Information Requirement (MIR) approach. Hydrologie dans le pays celtiques, Rennes (France), 8–11 Juillet, Ed. INRA, pp. 215–223.

Roth, D., Knoblauch, S., Pfleger, I., Herold, L., 1998. Nitratgehalte im Sickerwasser und N-Austrag aus unterschiedlichen Agrarstandorten Thüringens. Thüringer Landesamt für Landwirtschaft, Jena, Germany.

Shrestha, B.P., Duckstein, L., Stakhiv, E.Z., 1996. Fuzzy rule-based modeling of reservoir operation. J. Water Res. Plng. Mgmt. 122 (4), 262–269.

Smith, R.E., 1992. Opus, an integrated simulation model for transport of nonpoint-source pollutants at the field scale, vols. 1 and 2. US Department of Agriculture, ARS-98, Springfield, VA.

Srinivasan, R., Arnold, J.G., Muttiah, R.S., Walker, C., Dyke, P.T., 1993. Hydrologic unit model for the United States (HUMUS). In: Wang, S.S.Y. (Ed.), Advances in Hydro-Science and Engineering, vol. I. University of Mississippi, MS, pp. 451–456.

Young, R.A., Onstad, C.A., Bosch, D.D., Anderson, W.P., 1989. AGNPS: a nonpoint source pollution model for evaluating agricultural watersheds. J. Soil Water Conserv. 44 (2), 168–173.

Zimmermann, H.J., 1985. Fuzzy Set Theory and its Application. Kluwer Nijhoff Publishing, Dordrecht.