The SOIL-N/WEKU model system – a GIS-supported tool for the assessment and management of diffuse nitrogen leaching at the scale of river basins


* Research Centre Jülich, Programme Group Systems Analysis and Technology Evaluation (STE), D-52425 Jülich, Germany
** Department of Mathematics, Division of Statistics, Linköping University, SE-58183 Linköping, Sweden
*** National Environmental Research Institute (NERI), Vejlaevej 25, DK-8600 Silkeborg, Denmark

Abstract The SOIL-N/WEKU model system was developed to estimate groundwater-borne nitrogen inputs into river systems. The core of this model system is composed of a soil nitrogen leaching model (SOIL-N) and a groundwater residence time/denitrification model (WEKU). The application of the model system was carried out in the framework of the EU-project RANR (Regional analysis of subsurface nitrogen retention and its impact on the nitrogen export from land to sea) for a macroscale study river basin in Germany (the Uecker basin, ca. 2,400 km²) and a mesoscale study catchment area in Denmark (the Gjern basin, ca. 200 km²). For both catchment areas, the modelled average nitrogen loads leached into the groundwater were about 40 kg N/ha a, while the remaining groundwater-borne nitrogen intake to rivers was quantified to an average of about 2 kg/ha a. The comparison with observed groundwater-borne riverine nitrogen loads showed a very good agreement, proving the key role nitrogen retention in groundwater plays in the two catchment areas.

Keywords Denitrification in groundwater; diffuse nitrogen leaching; GIS – modeling; groundwater residence times

Introduction

All major processes involved in the turnover of nitrogen in soil and water have been thoroughly investigated by numerous scientists. Nevertheless, it has proved to be difficult to model large-scale phenomena, such as the riverine delivery of nitrogen from land to sea. Both environmental managers and scientists must admit that the inertia of the systems that control the loss of nutrients from land to sea was underestimated when the goal of a 50% reduction of the input of nutrients to the Baltic Sea and the North Sea was adopted.

The estimation of nitrogen fluxes through groundwater on the regional and supraregional scale requires approaches that can cope with the limited availability of input data at larger scales and yet describe complex processes. Many of the existing water quality models either do not explicitly focus on the spatial distribution of processes governing denitrification in groundwater (e.g. SPARROW: Smith et al., 1997), require very detailed three dimensional information about subsurface parameters (e.g. SWAT: Arnold et al., 1993) or are mainly applicable at the patch scale and in small homogeneous watersheds (e.g. OPUS: Smith, 1992).

In the present paper, we propose a new model system that is based on input data and mechanisms that are particularly relevant for the turnover of nitrogen at a spatial scale of river basins and a temporal scale of years to decades. The SOIL-N/WEKU model system is based on two different submodels particularly developed or adapted for this purpose, respectively. The two models are a regionalised version of the process-oriented and mechanistic one-dimensional soil nitrogen model (Soil-N-light) and the two-dimensional analytical groundwater nitrogen retention model (WEKU). The main objective of our study is to investigate the applicability of the SOIL-N/WEKU model system to estimate the long-term...
impacts of diffuse nitrogen pollution on groundwater nitrate load and retention in catchments.

Model system
The core of the proposed model system is composed of a soil nitrogen leaching model (SOIL-N) and a groundwater residence time/denitrification model (WEKU). A detailed description of the SOIL-N/WEKU model concept is given in Grimvall et al. (2001, in press).

Considering that agricultural land is normally the major source of the nitrogen carried by European rivers, we developed a module that describes the impact of agricultural production on the input of nitrate to groundwater. A process-oriented, one-dimensional soil nitrogen model (the SOIL-N model) was taken as a starting point in this work. The Soil-N model simulates major C and N-flows in agricultural soils and plants numerically. The model operates on a daily time step and simulates flow and state variables at field level (Johnsson et al., 1987). Basically, Soil-N-light describes how all nitrogen inputs to the soil-system, i.e. those from manure, inorganic fertiliser and atmospheric deposition either cause a change in storage pools, or leave the soil-system through crop harvesting, denitrification or nitrate leaching to groundwater aquifers. Given that all inputs to the soil-system as well as harvest are known, the total amount of nitrogen which is either denitrified or contributes to changes in the nitrogen storage pool have to be estimated to enable the calculation of nitrogen leaching.

The regionalised edition of Soil-N has been developed using statistical methods to identify the most important processes and parameters for long term nitrate leaching. The most important inputs to run Soil-N-light are the annual amount of Nitrogen-N added to the soil system from manure, inorganic fertiliser and from atmospheric deposition or removed from the soil system through crop harvest for up to 3 different soil types and up to 9 different crop classes. Extensive simulation studies were carried out to identify the factors or input variables that have the strongest impact on the (modeled) annual loss of nitrogen from the root-zone. In particular, it was revealed that meteorological conditions have a strong effect on the timing of the nitrogen leaching, whereas the time-averaged leaching of this element is almost exclusively determined by other factors. Further analysis of statistical relationships between model inputs and outputs showed that the nitrogen surplus (the difference between the application and deposition of nitrogen and the removal of this element with the harvest) is a natural starting point for estimating spatially and temporally aggregated root-zone losses of nitrogen. More precise leaching estimates can be obtained by employing the SOIL-N model to subtract estimates of nitrogen accumulation in soil organic matter and denitrification in the upper soil layers from the nitrogen surplus.

The mechanistic groundwater residence time model WEKU (Kunkel and Wendland, 1997) is used to calculate the periods of time taken by water from percolation into the groundwater-bearing rock up to its discharge into a surface water (river, lake, sea). The model is based on a velocity field generated from area-differentiated databases concerning the hydromechanical properties of the aquifers through which the water flows. It is assumed that the groundwater flow is always related to the upper aquifer. The WEKU model is using a stochastic approach to assess the influences of natural variabilities and uncertainties in the input data on the model results. Thus variation widths and confidence ranges for the calculated residence times can be quantified. Figure 1 gives a schematic overview of the general procedure and the databases required for WEKU residence time modelling.

Modelling is grid-based and essentially comprises two steps. In the first step the modelling input parameters hydraulic conductivity and effective yield of pore space of the aquifer
and the slope of groundwater surface (hydraulic gradient) are determined to quantify groundwater velocity according to Darcy’s law. The calculation of the residence times of the groundwater runoff is performed in a second step. Based on groundwater contour maps, a digital relief model of the groundwater surface is generated. This is analysed paying attention to information on the water network as well as the groundwater discharge or transfer areas with respect to lateral flow dynamics and groundwater-effective recipients. The residence times of the groundwater runoff are then obtained for each initial grid by summation over the individual residence times in the grids resulting from the groundwater velocities and individual flow distances along the flow path until they enter a surface water.

In the framework of this project the WEKU model was extended by a module for the quantification of nitrate degradation in groundwater. According to extensive field studies by Böttcher et al. (1989) in a catchment area in the North German Lowlands, and by van Beek (1987) for a site in the Netherlands, a first order denitrification kinetics has been assumed with a reaction constant in the range of 0.17 to 0.56 a⁻¹. This corresponds to a halving of the nitrogen leached to the groundwater after a residence time between 1.2 and 4 years. Quite simple indicators, such as the presence of Fe(II) and Mn(II) and the absence of O₂ and NO₃, can be used to decide if a groundwater province has hydrogeochemical conditions in which denitrification is possible or if such transformation of nitrogen can be neglected (Wendland and Kunkel, 1999).

Case study results and discussion

As case study regions we selected the Uecker basin with a catchment size of about 2,400 km², which is located in the extreme north-eastern part of Germany and the Gjern basin, which is located in the central part of Denmark and has a catchment size of about 200 km². A detailed description of the case study results is given in Grimvall et al. (in press). In Figure 2 the geographical location of the catchment areas and the groundwater residence times determined according to the WEKU-model are shown.
Groundwater residence times

The residence times shown in Figure 2 specify the time period that is required by the groundwater runoff fraction to proceed from the site of percolation into the groundwater up to the respective groundwater-effective recipient in the two basins. Depending on the site conditions, residence times ranging from less than one year to more than 150 years must be assumed. Long residence times may result both from small groundwater velocities as well as from long flow paths up to the recipient. Short residence times generally result for areas in the vicinity of rivers and/or regions with high groundwater velocities. The evaluation of the relative and the accumulated frequencies of the groundwater residence times for the Uecker basin showed that the median of the residence times is approx. 20 years, while about 75% of the calculated residence times are less than 80 years and 25% less than 6 years. For the Gjern basin the calculated median is 37 years, while 25% of the calculated residence times are below 12 years and 25% above 118 years.

As the groundwater residence times have an important impact on the nitrogen retention in groundwater and thus on the export of nitrogen from land to sea special efforts have been undertaken to validate the calculated values. This has been done using observed chloro-fluorocarbons (CFC) concentrations as reference values. The atmospheric source for CFC is relatively well known (e.g. refrigerants) and its concentration in the atmosphere has increased almost linearly from the 1940s to the late 1990s. Assuming that recharged groundwater is in equilibrium with the atmosphere, a measured CFC concentration in water can be converted to a corresponding atmospheric concentration, which in turn can be used to compute a corresponding date of recharge. The difference between the date of recharge and the date of sampling is the apparent age of the groundwater (Goode, 1999). Laier (1999) investigated the CFC-concentrations in the groundwater of the Gjern basin at four different sites (see Figure 2) and derived the according groundwater ages. The comparison of the calculated WEKU groundwater residence times versus the observed ages of groundwater (Laier, 1999) are listed in Table 1. The overall agreement between the observed values and the calculated groundwater residence times given by the WEKU model is very satisfying for the four sites. Thus we conclude, that the WEKU model gives reliable estimations for the groundwater residence times.

![Figure 2](https://iwaponline.com/wst/article-pdf/45/9/285/425660/285.pdf)

**Figure 2** Calculated groundwater residence times in the upper aquifer for the Uecker and Gjern basins
Denitrification conditions in groundwater

The analysis of the denitrification conditions in the groundwaters of the two river basins was done separately for the different groundwater bearing formations occurring in the catchment areas (moraine deposits, glacial outwash sediments). In total about 850 groundwater samples were evaluated and classified with respect to their nitrate-degrading capacity primarily on the basis of groundwater quality data on iron(II), manganese(II), oxygen and nitrate.

More than 75% of the sampling points in the hydrogeologic units occurring in the Uecker basin display oxygen concentrations below 2 mg O₂/l, indicating that the hydrogeological lithologic units can be classified as belonging to the predominantly reduced aquifers, in which denitrification may occur. As can be seen, iron(II) concentrations above 0.2 mg Fe(II)/l and manganese(II)-concentrations above 0.05 mg Mn(II)/l occur for roughly 90% of the sampling points. This is a further indication that the aquifers display predominantly reduced groundwaters and have a significant nitrate degradation capacity. At least more than 80% of the observed nitrate concentrations in the groundwater of both catchment areas are below 1 mg NO₃/l. In connection with the high iron(II) and manganese(II) and low oxygen contents, this is an indication that nitrate compounds leached out of the soil can be degraded in the groundwater systems. For the Gjern basin the evaluation of the groundwater monitoring data gave similar results. Hence, from the evaluation of the groundwater quality data for the Uecker and the Gjern basins it was expected that denitrification processes in the groundwater will take place. Accordingly we assume that diffuse nitrogen intakes will be reduced during the residence time of the groundwater in the aquifers.

Nitrogen leaching from the root zone

The actual nitrogen balance of the soils was analysed with the soil-N model using agricultural statistical data from both catchment areas. The long-term nitrogen balance averaged over several vegetation periods was calculated, considering the organic nitrogen fertilization, mineral nitrogen fertilization N fixation, atmospheric N inputs and N extractions with the crop substance as parameters. The summarized N-balance resulted for both basins in nitrogen surpluses in a range between ca. 30 kg N/ha a and 120 kg N/ha a. However, the nitrogen surplus is in general not equal to the nitrogen leached from the root zone to the groundwater systems. Within the SOIL-N model a certain fraction (up to 50%) is determined, which quantifies denitrification rates in the root zone as a function of soil properties and crop types. Additionally it has to be taken into account, that not all the nitrogen leached from the root zone reaches the surface waters via groundwater runoff. A certain fraction of the nitrogen leached from the root zone is coupled to the direct runoff components. In both catchment areas the ratio of direct runoff varies between 25 and 75%. On average, direct runoff accounts for ca. 30% of the total runoff. Whereas hence in most regions groundwater runoff is dominant, some sub-regions, i.e along the river valleys,
reveal high direct runoff fractions. In order to separate the fraction of nitrogen leached to groundwater from the total nitrogen leached from the root zone, the total nitrogen leaching from the root zone is weighted by the base flow ratio calculated according to Kunkel and Wendland (1998) for the Uecker basin and Kronvang et al. (1999) for the Gjern basin. The results are shown in Figure 3 and are similar for both catchment areas. High to very high nitrogen leaching to the groundwater of more than 40 kg N/ha a was calculated for all regions with a high groundwater runoff fraction and an intensive agricultural use on fertile luvisol soils. Regions with relatively low nitrogen intakes to the groundwater are obtained for areas where either less fertile soils and/or high direct runoff fractions predominate. Averaged over all agriculturally used areas the remaining nitrogen leaching from the root zone is quantified to 30 kg N/ha a for the Uecker basin, and to 26 kg N/ha a for the Gjern basin.

Groundwater-borne nitrogen inputs into surface waters

In Figure 4 the remaining nitrogen inputs into the surface waters from groundwater runoff after transport and denitrification in the aquifer are shown. As can be seen, in most areas of the two basins nitrogen is almost completely removed during the transport in the aquifer to surface waters. Only nitrogen intakes in the vicinity of surface waters and high nitrogen leaching levels contribute considerably to the nitrogen loads of rivers. The average groundwater-borne nitrogen input into the Gjern and the Uecker was quantified to about 2 kg N/ha a. The comparison of this value with the average nitrogen load leached from the root zone (Figure 3) indicates that through denitrification in the groundwater more than 90% of the nitrogen inputs into groundwater are retained in the aquifer systems of the two basins.

The modelled nitrogen inputs into surface waters from groundwater have been compared to observed nitrogen concentrations in rivers under base flow conditions (e.g. Behrendt et al., 1999). The values calculated with the combined SOIL-N/WEKU model only show relatively small differences to the observed values (about 10–20%). This can be regarded as a very good agreement.
Conclusions

Studies of selected catchments in Denmark and Germany showed that both the groundwater residence time and the amount of nitrogen that is denitrified can vary strongly with the site in which the nitrogen enters the saturated zone. This may explain why there is sometimes an unclear water quality response to changes in land use. In principle, long groundwater residence times and favorable conditions for denitrification may also be responsible for the delivery of low groundwater-borne nitrogen loads to the surface waters in the Uecker and the Gjern basins. From the results of the case studies for the two river basins we conclude that about 90% of the diffuse nitrogen input into the groundwater is degraded in this way. The comparison with observed groundwater-borne riverine nitrogen loads proves the reliability of the modeled values. Thus we conclude that the combined SOIL-N/WEKU model was applied successfully for the quantification of groundwater-borne nitrogen leaching to surface waters in the two catchment areas.

With regard to the supraregional (e.g. European) perspective however, the two catchment areas are relatively small. This raises the question whether it is possible to generalize and transfer the SOIL-N/WEKU model to other regions. In this connection it is important that the two basins are about 500 km distinct from each other. Nevertheless the Gjern and the Uecker basins are located in the same supraregional geological structure of the European Pleistocene Lowland, which ranges from the Netherlands in the west and Denmark in the north to the Baltic States and the Ukraine in the east. As could be shown, the key factors controlling the subsurface nitrate retention (residence times, denitrification capacity) are correlated to specific hydrogeological site conditions, occurring in the Uecker as well as in the Gjern basin. Studies carried out by Kunkel and Wendland in the northern part of the Elbe basin (ca. 60,000 km²), which is geographically located between the Uecker and the Gjern basin and is a part of the European Pleistocene Lowland too, showed an equal distribution of groundwater residence times (Kunkel and Wendland, 1999) as well as the same hydrogeochemical characteristics (Wendland and Kunkel, 1999). With regard to the European perspective we would assume on the basis of these results that “long” residence times and “good” denitrification conditions should in general be valid for the entire European Pleistocene Lowland. Consequently we think that the transfer and application of...
the SOIL-N/WEKU model concept to other catchment areas in this supraregional geological structure should be possible without major problems. The advantage of such a broader application of the SOIL-N/WEKU model concept would lie in the supraregional quantification of the role subsurface nitrogen retention may play in the entire Pleistocene European Lowland. In the same way, it would be possible to evaluate sensitive regions inside this supraregional structure, i.e. areas with high nitrogen surpluses and low groundwater residence times and hence incomplete subsurface nitrogen retention. However it has to be taken into account, that this estimation is at the present stage no more than a rough estimate on the basis of the results from our study and on knowledge about the general geological structure in Europe. Statements about the applicability of the combined SOIL-N/WEKU model for these areas can only be proved in the course of further selective studies.

References