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# Modelling of N-movements on catchment scale – a tool for analysis and decision making.

## 1. *Model description*

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*Key words:* catchment scale, simulation model, soil water dynamics, soil nitrogen dynamics, unsaturated and saturated zone

**Abstract**

The aims of the study were to describe 1) the overall relationship between additions of nitrogen (as fertilizer and manure) to the ground surface and the nitrate concentrations in groundwater and streams, as well as 2) the consequences of changes in agricultural management practices. A mathematical modelling system has been established, which comprise two models, 1) a physically-based rootzone model (DAISY) for simulation of the nitrogen dynamics in the rootzone, and 2) a physically-based and fully distributed catchment model (MIKE SHE) for simulation of the water and solute transport in a catchment. The modelling system includes the nitrate transformations in the rootzone and at the redoxcline in the aquifer. Nitrate movement is described from application on the field to its occurrence in the stream.

The article describes the modelling system and the data requirements. The model was tested on the 425 $km^2$ Karup stream catchment. Inputs used and results of simulations with the system are given in part II (this issue).

## Introduction

During the last decade, an increasing nitrate load has been registered in the groundwater, streams, lakes, and fjords of Denmark. Most of this nitrate is thought to originate from non-point pollution from agricultural areas, following increased use of animal manure and fertilizer.

Although a large number of detailed studies of specific processes of nitrogen transformations and movement in soil have been carried out (Addiscott, 1983; Groot and Verberne, 1991; Rolston *et al.*, 1984; Veen *et al.*, 1984), integrated modelling analyses of the fate of nitrogen from its application to the fields to the appearance as nitrate in surface waters are scarce. The models developed have usually been confined to specific parts of the hydrological system of a catchment, e.g. either the root zone or the groundwater zone alone.

ANIMO (Berghuijs *et al.*, 1985; Jansen, 1991), DAISY (Hansen *et al.*, 1990) and SWATNIT (Vereecken *et al.*, 1990) are examples of mathematical models developed to describe nitrate uptake and movement in the root zone (a soil column), but they do not include movement or transformation in groundwater. A large number of N-root zone models have been reviewed by other authors (Vachaud *et al.*, 1988; Willigen *et al.*, 1988), while comparative tests of five N-root zone models were carried out under the auspices of the EEC (CEC, 1991).

A large number of complex groundwater models exist, which include a physically-based representation of the physical and chemical processes of contaminant transport in groundwater (see e.g. Kinzelbach and Schäfer, 1991). These models have in general not been linked with agricultural models to include the transformation and transport taking place in the unsaturated zone from non-point pollution sources. Bogardi *et al.* (1988) have reviewed models describing the effect of agricultural non-point pollution on groundwater quality, concluding that the art is still in its infancy, with most of the work done on simple conceptual models. One of the most sophisticated modelling approaches presented in the review is the use of the N and organic Carbon-model ANIMO combined with the water management model SIMGRO (Querner, 1988). ANIMO considers soil type, land use, water management, weather conditions, fertilizer use and cropping history, while SIMGRO simulates flow in the saturated and unsaturated zones in a quasi-three-dimensional way (i.e. the model describes the flow two-dimensionally in several layers, the exchange between layers being determined by explicit sink-source-terms).

The purpose of the present study has been to perform a detailed modelling analysis of N-transformations and transport in a medium-sized catchment through a coherent three-dimensional deterministic modelling system. This type of modelling can be helpful in the decision-making process to evaluate the effects of either regional or local management strategies on the regional groundwater system or other recipients e.g. the stream system. Whereas detailed studies at field scale are useful for analysing processes and development of models, regional studies provide a better basis for producing extrapolations to larger regions or even at national scale.

In this paper, the modelling system and the data requirements are described. Examples of results from a case study may be found in Styczen and Storm (1993).

## The mathematical modelling system

The modelling system consists of two separate models, the DAISY model and the MIKE SHE modelling system.

### *The MIKE SHE modelling system*

MIKE SHE is a fully distributed hydrological catchment model that calculates the flow of water and solutes in the catchment by solving the governing equations of overland and channel flow, and unsaturated and saturated flow, by finite difference methods. The model is completed by the processes of snow melt, canopy interception, and evapotranspiration. MIKE SHE (Danish Hydraulic Institute, 1993; Storm *et al.*, 1990) is an extension of the original SHE modelling concept described in (Abbott *et al.*, 1986a,b)

The variation in catchment characteristics (e.g. land use, soil, geology, topography and river geometry) and driving variables (e.g. climatic input data) are represented in a network of squares in the horizontal direction. Each square is further subdivided into a number of layers in the vertical direction to describe variations in the soil profile and the groundwater aquifer system.

The vertical flow in the unsaturated zone is described by the one-dimensional Richard's equation independently for each square. The soil columns thereby link the three-dimensional groundwater flow system to the two-dimensional flow system for overland flow. Lateral unsaturated flow between the soil columns is neglected since this phenomenon is insignificant under normal conditions. The channel system is assumed to run along the boundaries of the grid squares (links). The channel routing is solved by the one-dimensional diffusive wave approximation of St. Venant's equation (Abbott, 1979). At each link the river receives lateral groundwater and overland inflow from the adjacent squares. The structure of MIKE SHE is illustrated in Figure 1. Utilizing the velocities of the water computed by solving the above equations, the advection and dispersion of the solutes in the catchment is calculated by solving the appropriate advection-dispersion equations.

### *The DAISY model*

DAISY (Hansen *et al.*, 1990; 1991) is a one-dimensional, physically-based root zone model, which simulates crop production, soil water dynamics and nitrogen dynamics under various agricultural management practices.

The hydrological processes considered in

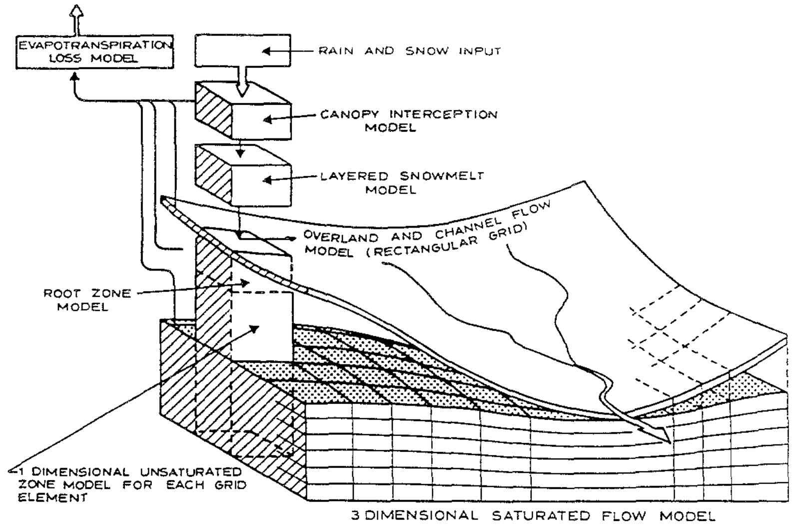


*Fig. 1.* The structure of the MIKE SHE modelling system.

DAISY include snow accumulation and melting, interception of precipitation by the crop canopy, evaporation from crops and soil surface, infiltration, water uptake by plant roots, transpiration, and vertical movement of water in the soil profile. The model uses an identical numerical solution scheme for solving Richard's equation to the unsaturated zone component of MIKE SHE, and is therefore under many conditions compatible with MIKE SHE in the unsaturated flow description. DAISY uses a flux boundary, a fixed groundwater level or a file of groundwater levels as lower boundary condition.

The transformation and transport processes considered in DAISY include net mineralization of nitrogen, nitrification, denitrification, nitrogen uptake by plants and nitrogen leaching from the root zone. Mineralization is determined by the turnover of three organic matter pools. Each pool is divided into two or three sub-pools, characterized by C/N-ratio and turnover rate. Nitrification depends on soil temperature and soil water status, and is described by 1st order kinetics. Denitrification is governed by soil temperatures, soil water status, and oxygen content. Nitrogen uptake by plants is determined as the nitrate flux to the root surface, governed by mass flow and diffusion, which in turn depend on the concentration-distance profile around the roots.

Nitrogen in various forms may be added as atmospheric deposition, fertilizer, different types of animal manure, or plant residues. Furthermore, the model contains a soil temperature module and a crop growth model (growth limited by water and/or N availability).

### *The combined system of MIKE SHE and DAISY*

By combining the two models, a complete mathematical modelling system is available, which can simulate the water and nitrate transport in the catchment including the transformation processes in the root zone (Fig. 2).

The two models are running sequentially. First MIKE SHE is calibrated at catchment scale by obtaining acceptable agreement between simulated and observed spatial and temporal variations in runoff and groundwater heads in the catchment. This also ensures a correct simulation of temporal and spatial distribution of recharge to the groundwater. In the initial calibration phase assessed and standardized crop parameters (time series of LAI and root development) are used in the simulations. These are later modified according to the simulated values obtained from the DAISY model.

Time series of daily crop status (LAI and root development) and daily mass of nitrate leaching (in kg $ha^{-1}$) are simulated with DAISY for all combinations of cropping sequences and corresponding estimates of fertilizer, manure applica-

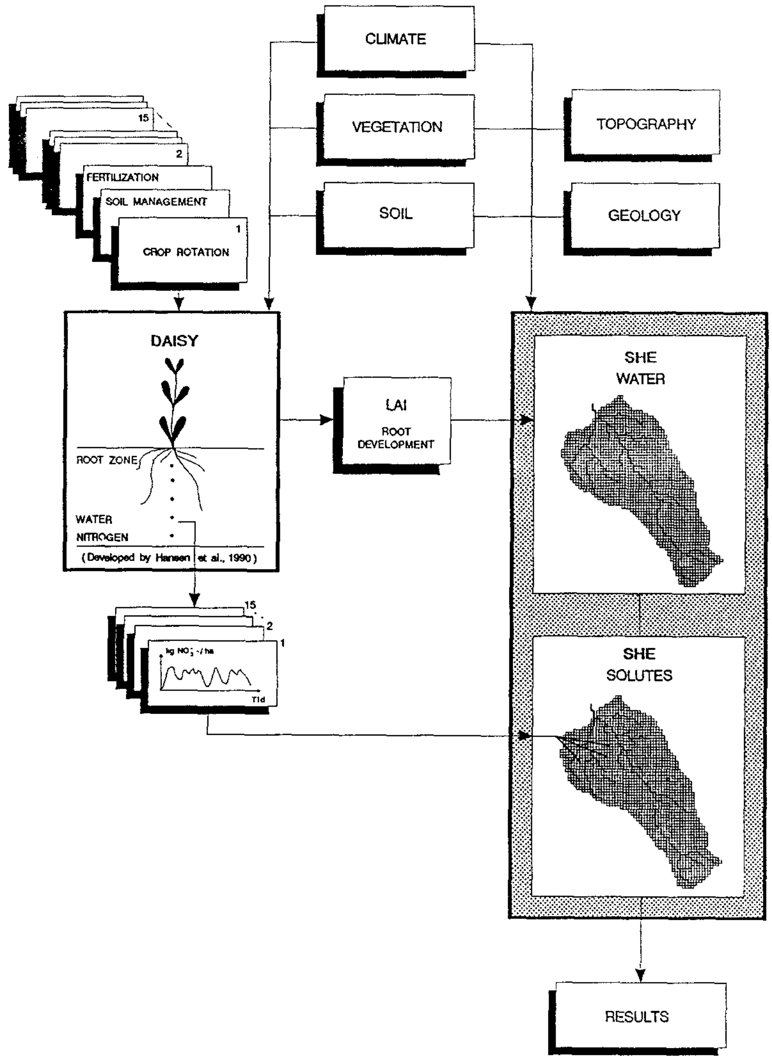


*Fig. 2.* Schematical representation of the data requirements for the two models and the linkage between them.

tions and management practices, identified in the catchment.

These are then distributed across the MIKE SHE grid according to their occurrence. The generated crop status parameters are used in MIKE SHE to recalculate the water flow and to ensure full compatibility in the recharge volumes between DAISY and MIKE SHE. The daily nitrate (mass) leaching at 1.2 m depth is used as input in the advection-dispersion module of MIKE SHE.

As denitrification plays only a minor role in the well-aerated unsaturated zone below the root zone, nitrate is treated as a non-reactive solute in this part of the hydrological regime. Below the groundwater table, strong denitrification was observed in a parallel study (Postma and Boesen, 1991) of the catchment of Karup stream, Jutland. The conditions change from oxidized to reduced at certain depths in the aquifer, as illustrated in Figure 3. This boundary is termed the redoxcline. For the groundwater zone, a simple formulation assuming that all nitrate reaching the redoxcline is removed instantaneously was therefore introduced in MIKE SHE. This simple formulation was based on the findings (Postma and Boesen, 1991) that the redoxcline in the study catchment moves slowly downwards (approx. 2 cm/year) due to a high buffer capacity of the aquifer and the flow

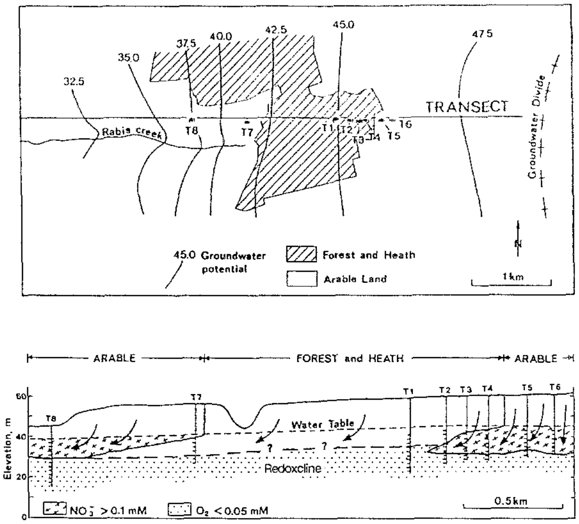


*Fig. 3.* Assumed position of redoxcline in the Rabis Brook subcatchment based on well logs. Modified from Postma and Boesen (1990).

pattern. During the time scale under study this was assumed negligible.

Because of the significant and spatially varying denitrification, which takes place in the aquifer, it is very important to simulate groundwater movement in a three dimensional manner to estimate the total amount of nitrate that reaches the stream system and to determine from which part of the catchment it originates.

## Data requirements

Daily values of the following weather variables are required for the two models:

| | DAISY | MIKE SHE |
|---|---|---|
| Precipitation | x | x |
| Temperature | x | x |
| Potential evapotranspiration | x | x |
| Global radiation | x | |

While DAISY uses a specific set of soil parameters for each simulation, MIKE SHE requires a description of the spatial distribution of each soil type in the catchment. Both models require the soil moisture characteristic and a hydraulic conductivity function (or just the saturated hydraulic conductivity) for each soil horizon in a profile. In addition, DAISY requires information on texture and the maximum allowed rooting depth. With respect to chemical properties, DAISY requires information on total C content, and C/N in different depths in the soil, the partitioning of C and C/N in pools, and the initial content of nitrate or ammonia in the soil. The initial contents of nitrate and ammonia mainly influence the simulations during the first year, and lack of data can be overcome by running the model through a 'warming up year'. Transformation rates for the different pools, parameters for dispersivity and impedance, ammonia isotherms, and parameters for denitrification are determined from experiments and are usually kept constant for different model applications.

MIKE SHE requires information on the spatial distribution of different vegetation types, and estimates of root depth and leaf area index (both as functions of time). DAISY generates root depth and leaf area index from information on type of crop, sowing and harvesting dates, tillage practices, irrigation, and fertilizer/manure applications. For mineral fertilizer, application method, total N-content and ammonia-content must be specified. For organic manure, also dry matter and C-content should be supplied. To calculate the amount of crop residues correctly it should be specified which parts of the crop are harvested and which are left, or parameters such as harvest index and stubble dry matter should be given. In addition, rates for dry and wet deposition of N are given as inputs.

MIKE-SHE requires a description of topography and drainage pattern. For the streams, cross sectional geometry and roughness coefficients are inputs.

Depending on the particular site and the required depth of simulation, DAISY may need information on the groundwater table (constant or varying). MIKE SHE needs information on the groundwater table as part of the initial conditions. However, MIKE SHE requires information on the extent of geological layers, and for each layer, the horizontal and vertical saturated hydraulic conductivity and storage coefficient (unconfined and confined). In case groundwater extraction takes place, the location of wells and depth of screens are required.

MIKE SHE is calibrated on data such as river discharges (one or several stations), groundwater heads and soil moisture at selected points (if available).

DAISY can be calibrated on measurements of either soil moisture or tension (or both), as well as nitrate concentrations in soil moisture.

## Conclusion

By combining the DAISY model with the MIKE SHE modelling system, a comprehensive three-dimensional modelling system has been developed, allowing analysis of N-transformations and transport in a catchment. Results of a case study, where the model has been applied and comparisons to measurements are described in Styczen and Storm, 1993 (this issue).

## References


Abbott MB (1979) Elements of the Theory of Free Surface Flows. Pitman, London.

Abbott MB, Bathurst JC, Cunge JA, O'Connell PE and Rasmussen J (1986) An introduction to the European Hydrological System. 1. History and philosophy of a physically-based distributed modelling system. J Hydrol 87: 45–59

Abbott MB, Bathurst JC, Cunge JA, O'Connell PE and Rasmussen J (1986) An introduction to the European Hydrological System. 2. Structure of a physically-based distributed modelling system. J Hydrol 87: 61–77

Addiscott TM (1983) Kinetics and temperature relationships of mineralization and nitrification in Rothamsted soils with different histories. J Soil Sci 34: 343–353

Berghuijs JT -van Dijk, Rijtema PE and Roest CWJ (1985) Animo – Agricultural nitrogen model. Institute for Land and Water Management Research, Wageningen. Nota 1671.

Bogardi I, Fried JJ, Frind E, Kelly WE and Rijtema PE (1988) Groundwater quality modelling for agricultural nonpoint sources. In: DeCoursey DG (ed) Proceedings of the International Symposium on Water Quality Modelling of Agricultural Non-Point Sources, June 19–23, 1988, Utah State University, Logan, Utah. USDA, ARS81: 227–253

CEC (1991) Soil and groundwater research report II. Final Report, contract nos. EV4V-0098-NL and EV4V-00107-C. EUR 13501.

Danish Hydraulic Institute 1993 MIKE SHE Short Description. Hørsholm, Denmark.

Groot JJR and Verberne ELJ (1991) Response of wheat to nitrogen fertilization, a data set to validate simulation models for nitrogen dynamics in crop and soil. Fert Res 27: 349–383

Hansen S, Jansen HE, Nielsen NE and Svendsen H (1990) DAISY: A soil plant system model. Danish simulation model for transformation and transport of energy and matter in the soil plant atmosphere system. NPo Research in the NAEP, Report A10. National Agency of Environmental Protection, Copenhagen, Denmark.

Hansen S, Jensen HE, Nielsen NE and Svendsen H (1991) Simulation of nitrogen dynamics and biomass production in winter wheat using the Danish simulation model DAISY. Fert Res 27: 245–259

Jansen EJ (1991) Brief description of the nitrogen model ANIMO. In: CEC (1991) Soil and groundwater research report II. Final Report, contract nos. EV4V-0098-NL and EV4V-00107-C. EUR 13501.

Kinzelbach W and Schäfer W (1991) Numerical Modelling of Natural and Enhanced Denitrification Processes in Aquifers. Water Resour Res 27: 1123–1135

Postma D and Boesen C (1990) Nitrate reduction processes in the aquifer of the moreland plain of Rabis, Groundwater chemistry and modelling. NPo Research in the NAEP, Report B8. National Agency of Environmental Protection, Denmark. (In Danish)

Postma D and Boesen C (1991) Nitrate reduction in an unconfined sandy aquifer: Water chemistry, reduction processes and geochemical modelling. Water Resour Res 27: 2027–2045

Querner EP (1988) Description of a regional groundwater flow model SIMGRO and some applications. Proceedings Symp. Agrohydrology, Sept. 29-Oct. 1, 1987. Agricultural Water Management, Special Issue 14: 209–218

Rolston DE, Rao PSC, Davidson JM and Jessup RE (1984) Simulation of denitrification losses of nitrate fertilizer applied to uncropped, cropped and manure-amended field plots. Soil Science 13: 170–279

Storm B, Styczen M and Clausen T (1990) Regional model for nitrate transport and transformation. NPo Research in the NAEP, Report B15. National Agency of Environmental Protection, Copenhagen Denmark. 120 p (In Danish)

Styczen M and Storm B (1993) Modelling of N-movements on catchment scale – a tool for Analysis and Decision Making. II. A case study. Fert Res 36: 7–17

Vachaud G, Vauclin M and Addiscott TM (1988) Solute transport in the vadose zone: A review of models. In: DeCoursey DG (ed) Proceedings of the International Symposium on Water Quality Modelling of Agricultural Non-Point Sources, June 19–23, 1988, Utah State University, Logan, Utah. USDA, ARS81: 81–104

Veen JA van, Ladd JN and Frissel MJ (1984) Modelling C and N turnover through the microbial biomass in soil. Plant Soil 76: 257–274

Vereecken H, Vanclooster M and Swerts M (1990) A model for the estimation of nitrogen leaching with regional applicability. In: Merckx R, Vereecken H and Vlassak K (eds) Fertilizer and the Environment. Proc of the Int. Congress on Fertilizer and the Environment, pp 250–263. Leuven Academic Press, Leuven, Belgium

Willigen P de, Bergström L and Gerritse RG (1988) Leaching of the unsaturated zone: Their potential use for management and planning. In: DeCoursey DG (ed) Proceedings of the International Symposium on Water Quality Modelling of Agricultural Non-Point Sources, June 19–23, 1988, Utah State University, Logan, Utah. USDA, ARS81: 105–128