Non-point pollution modelling at different scales and resolution, based on MIKE SHE

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Abstract

The spread of tools for assessing the contribution of non-point pollution to groundwater or surface water systems range from very simple to very advanced models. The simple models do not, in general, take into account the annual variations in weather and they are seldom able to incorporate effects of management in a realistic manner. The advanced models require extensive parameterisation. Furthermore, important decisions are required regarding the size of area, the resolution (grid size) used in the model, and the level of details required for the input. The article provides an overview of strategies used at the Danish Hydraulic Institute in non-point pollution modelling when different scales are considered, moving from small study areas to small catchments to regional scale or vice versa. These strategies were applied in former and ongoing projects. Furthermore, effects of different resolutions on a given catchment are exemplified. The influence of the level of detail in the data source can be evaluated from two studies carried out.

In general, scaling up with respect to size of area (of similar type) can be done with reasonable results for nitrate. Simulations of a particular catchment with a given set of base data, but with different grid resolutions, demonstrates that the simulated river discharge hydrograph strongly depends on the grid resolution, whereas annual discharge values and aquifer nitrate concentrations are less dependent on grid resolution. Regarding data resolution, the experience with regional databases is not unidirectional. For areas with little variation in landscape factors, regional simulations of nitrate concentrations in groundwater were adequate. For more complex areas, particularly due to a more complex geology, the information was inadequate.

1 Introduction

DHI's experience in non-point pollution modelling mainly relates to nitrate and pesticides. The involvement in non-point pollution modelling began in 1990, with modelling of nitrate at catchment scale under the Danish "Nitrate, Phosphorus, and organic matter" research programme. The programme was a consequence of the increasing eutrophication observed in the coastal zone of Denmark, but also in lakes, streams and to some extent in groundwater.

The work on nitrate modelling was (and is) done in close co-operation with the Royal Veterinary and Agricultural University in Copenhagen, who developed the DAISY-model for nitrate modelling. The experience gained was later used in other projects in Denmark and

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Slovakia, and DHI is presently involved in nitrate modelling in Poland and at another Danish site. A common feature of the projects has been calibration of model components on plot scale or at least on small catchments along with upscaling to larger areas.

The major strength of the advanced N-modelling in comparison to simple estimates is the possibility of evaluating effects of farm management changes on nitrate leaching. In addition, comparison between simulations and measured data allows distinguishing between effects of management and effects of weather.

The work on modelling of transport and transformation of pesticides started a few years later, and has, until recently, concentrated on simulation of single columns (point scale). However, as the ongoing national monitoring programme documents presence of pesticides in groundwater and surface water, the need for modelling of pesticide dynamics in at least small catchments has grown.

2 Models

The non-point pollution modelling conducted by DHI has involved the use of the hydrological model system MIKE SHE (Abbott et al., 1986 a,b; and Refsgaard and Storm, 1995). MIKE SHE functions as a catchment-modelling tool, able to simulate flow and solute transport. Different modules describing the reactions of the solutes are then added to this description.

For pesticides, these process descriptions have been implemented as part of the MIKE SHE system from the beginning. For nitrate it has been different: In the beginning, the DAISY model, developed at the Danish Veterinary and Agricultural University, so closely produced the output of the unsaturated zone, subsequently transferred as input to the MIKE SHE system. Recently, the two models were integrated, so the reactions and temperature calculations take place in DAISY while the flow and solute transport take place in MIKE SHE. With respect to pesticides, another recent development is a further merging between the DAISY process descriptions and the pesticide processes: A module for microbiological degradation and sorption in MIKE SHE utilises the organic matter turn-over of DAISY to regulate pesticide turn over, also determined by redox conditions.

It is a causcious decision to link MIKE SHE and the DAISY model. DAISY has proven its quality in several model inter-comparisons, and its performance under Danish conditions is well documented. It is being maintained in its stand-alone form by the University, and is thus continuously updated, as new results become available. Essentially, the aim is to work with few model codes with a high degree of flexibility, in order to be able to cover as many practical situations as possible.

2.1 MIKE SHE

MIKE SHE is at present the only physically based, dynamic, fully distributed modelling tool for integrated simulation of all major hydrological processes occurring in the land phase of the hydrological cycle. The combination of a physically based and a distributed model enables a direct use of field data for model building and it enables linking to spatial data that may, for instance, be provided through remote sensing or fields survey programmes. The integrated approach makes MIKE SHE suitable for simulation of hydrologic systems where surface water and groundwater interactions are significant.

The basic MIKE SHE module is the Water Movement module describing the hydrological processes. The hydrological components included are interception-evapotranspiration, infiltration, snow melt, 1-dimensional flow in the unsaturated zone, 3-dimensional ground water flow, overland flow in 2-dimensions and 1-dimensional river flow, all of which are fully coupled.

MIKE SHE can be combined with a variety of add-on modules used to address specific environmental problems among these solute transport by advection and dispersion (MIKE SHE AD). The integrated approach also covered by the solute transport and the module flexibility make MIKE SHE suitable for a large variety of environmental and hydrological issues. MIKE SHE is applicable on spatial scales ranging from a single soil profile to large regions, which may include several river catchments.

2.2 DAISY

DAISY is an advanced soil-plant-atmosphere system column model. It describes crop production as well as water and nutrient dynamics in the root zone of the agro-ecosystems according to various management strategies, including crop rotations, fertilisation, irrigation, soil tillage and crop residue management. The model simulates processes including: plant growth and crop production; heat flux and soil temperature; soil water uptake by plants and evapotranspiration; carbon and nitrogen mineralisation; nitrification and denitrification (nitrogen transformation); nitrogen uptake by plants.

Combined with the MIKE SHE WM and AD modules (*Figure 1*), the DAISY module provides a powerful tool for the assessment of the regional impacts of agricultural crop production system management on water quality conditions in the soil, the groundwater, and streams.

The DAISY module requires temporal information on air temperature and global radiation and information on humus and inorganic nitrogen content in the soil. As agricultural driving variables, information on crop rotations, tillage operations, fertilisation, and irrigation need to be specified at present. The DAISY module provides crop parameters for 12 crops, which are calibrated using data from crop varieties grown in northern Europe. To ensure that the crop development is simulated correctly, it may be necessary to recalibrate these parameters using local data on crop development.

The DAISY model is developed by the Royal Danish Veterinary and Agricultural University. Further development of the MIKE SHE DAISY is ongoing to include atmospheric processes and remote sensing. Additionally, phosphorus transformations and transport is expected to be included within a few years.

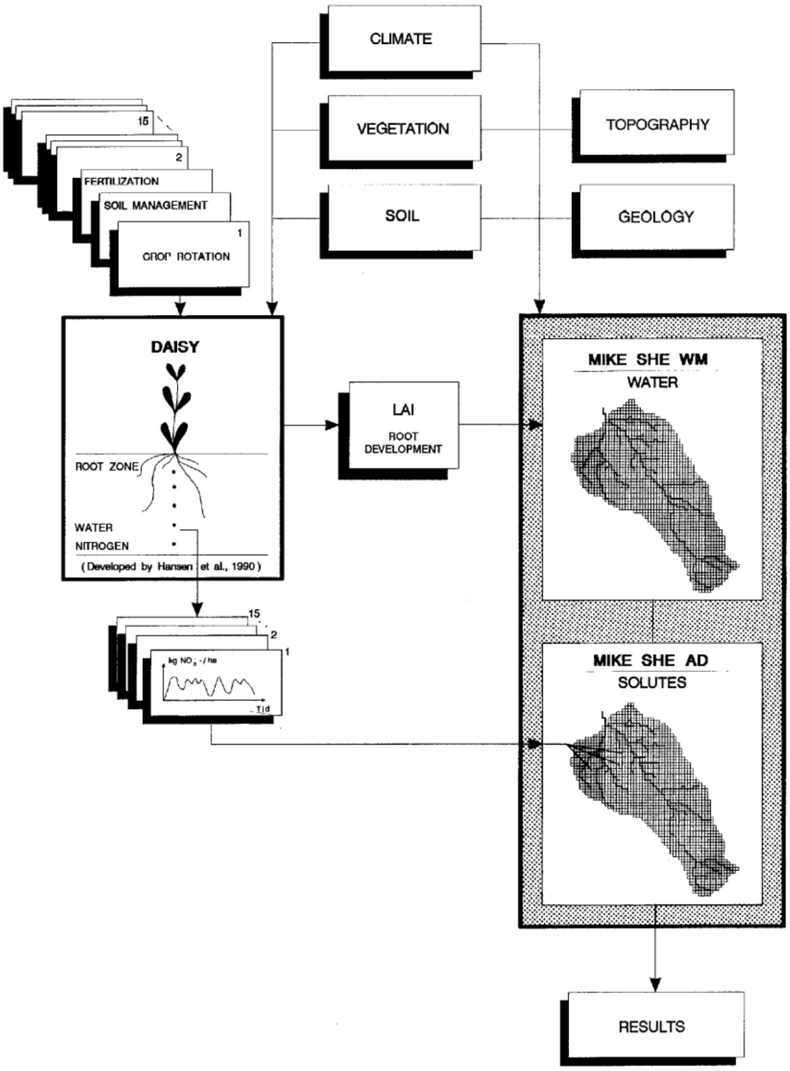


Figure 1 The integration between DAISY and MIKE SHE. DAISY simulates evaporation, infiltration, temperature, growth, and nitrogen transformations. MIKE SHE simulates transport of water and solutes.

2.3 Pesticide

Modelling the transport and metabolism of pesticides needs incorporation of sorption and degradation processes in the transport process. Besides the physical transport by advection and dispersion these two chemical and microbiological processes are the most influential regarding the transport and fate of pesticides.

The MIKE SHE sorption/degradation (SD) module includes simplified descriptions of complex geochemical and microbiological processes. In combination with the MIKE SHE AD module it constitutes a model tool for describing the influence on pesticide transport by chemical and microbiological processes. Both linear and non-linear equilibrium or kinetic sorption are options dependent on reaction rates and distribution coefficients for the pesticides. A first order process describes the microbiological degradation of the pesticides with a certain half-life time constant. This description of pesticide metabolism has been used earlier in projects and might be sufficient with respect to most problems.

The MIKE SHE geochemical module (GM) and biodegradation module (BM) includes advanced descriptions of complex geochemical and microbiological processes, respectively. The GM module handles all inorganic equilibrium chemistry (precipitation, dissolution, complexation, ion exchange, redox, and sorption) by invoking the PHREEQC code (Parkhurst, 1995). The BM module handles various biological processes (0. order, 1. order, Monod kinetics) and can be tuned to handle solute specific expressions derived from laboratory experiments. In combination with the MIKE SHE AD module these two modules constitute an advanced model tool for describing the influence on pesticide transport by chemical and microbiological processes. This model system is employed in the most recent studies of pesticides that require the most careful and accurate description of the metabolism, e.g. a study on pesticides and groundwater, Section 4.2.2.

3 Approach to Non-point Modelling

Large-scale hydrological models are required for a variety of applications in hydrological, environmental and land surface-atmosphere studies, both for research and for day to day water resources management purposes. The complex interaction between spatial scale and spatial variability is widely perceived as a substantial obstacle to progress in this respect (Blöschl and Sivapalan, 1995; and many others). The process of upscaling does pose problems, particularly if it is attempted to describe the processes differently, depending on the scale of application. The method, which has been applied at DHI, does not employ different process descriptions, but rather an aggregation procedure. In the aggregation to macro-scale, the variations in spatial data such as soil types and crops are preserved statistically, although they are not correctly georeferenced.

In all applications, the same modelling system is used whether the simulation represents field or plot scale, a small catchment or a region. However, the models differ with respect to area covered, resolution (grid size) and the level of detail available with respect to input data. All three factors influence the result of the simulation.

It is of outmost importance that the model code has been validated at plot scale, preferably under different conditions. This way it is ensured that the process descriptions are appropriate and that realistic results can be obtained with a physically relevant parameterisation. Figure 2 illustrates some of the complexities of non-point pollution pathways and scales. Plot scale means, in this sense, not necessarily point scale, but rather a field scale characterised by “effective” soil and vegetation parameters, but assuming only one soil type and one cropping pattern. Thus, the spatial variability within a typical field is aggregated and accounted for in the “effective” parameter values (Refsgaard et al., 1998). MIKE SHE and DAISY have documented their ability to describe conditions at field scale (e.g. Jensen and Refsgaard, 1991

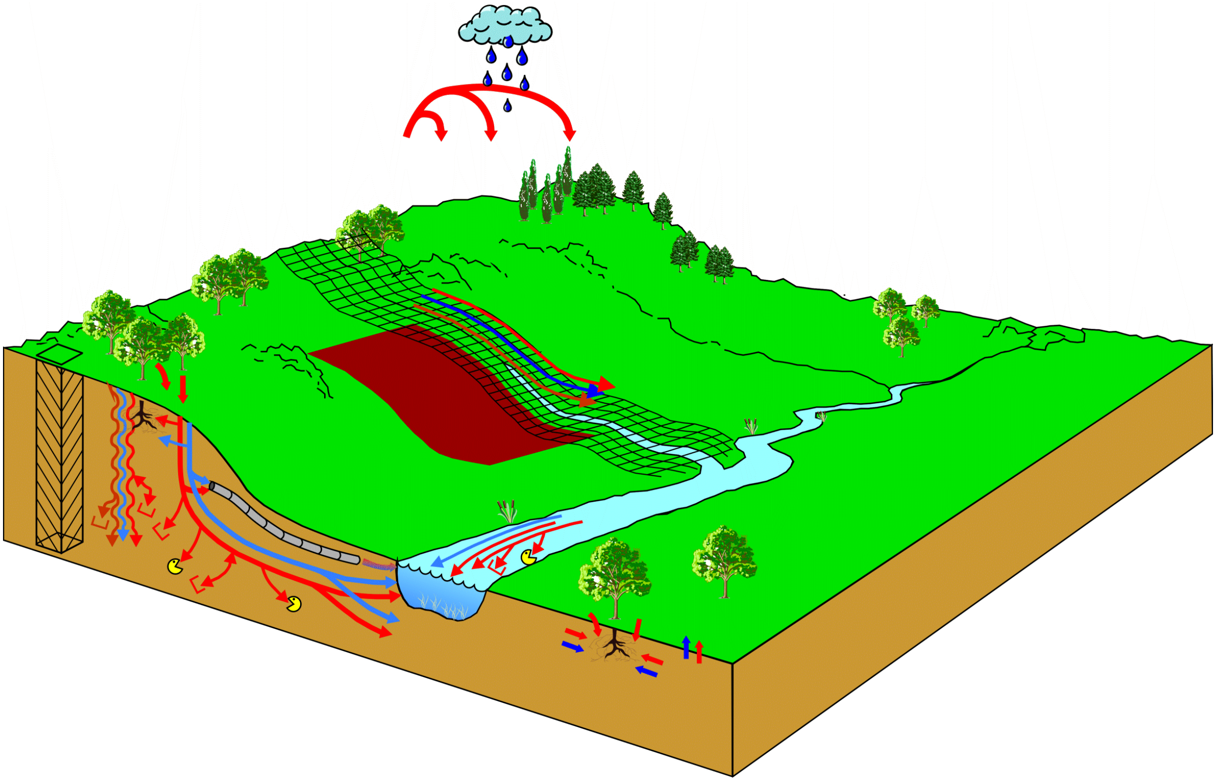


Figure 2. *Simulations of processes in a catchment may take place at plot, local or regional scale, symbolised by a soil column, a subcatchment or the whole area. Relevant processes for non-point pollution may include transport along the soil surface, through the soil matrix or macropores, in drains and in groundwater, of water (blue) and solute in soluble (red) or particle bound (brown) form, as well as several types of transformations.Transformations e.g. be degradation, plant uptake, or fixation through sorption or immobilisation. Some chemicals are subject to drift and volatilisation.*

a, b, c; Djurhuus et al., 1999; Svendsen et al., 1995, Diekkrüger et al., 1995; and Willigen, 1991).

For field or plot scale simulations measured data are employed to the largest possible extent. Calibrations are carried out on available data, such as soil moisture measurements, drain flow, or solute concentrations. It is a rule at all scales of simulations that the flow-relevant parameters are calibrated first (groundwater levels, drain flow, river flow, moisture in the soil profile), followed by calibration of conservative tracer, if data are available, and finally the chemical in question. A strong advantage of utilising one model system is that the implemented model can be tested on detailed data when these are available.

When moving to a small catchment, measured data are still utilised to the greatest possible extent, but it becomes necessary to generalise information into a number of types (soil, crop rotations, fertilisation times, etc.). The level of information available for a column is usually less than at the detailed level. The grid size is usually larger.

At the regional scale, the model parameters are based on best guesses constructed from statistical information, interviews, national databases, etc. Parameters calibrated from detailed studies will form the basis for qualified guessing, but the availability of precise information is (considerably) less than at the plot scale and generally less than in the small catchment. In principle, the grid resolution could be the same as for the small catchment. In practise, however, it will usually be larger. The grid resolution issue is discussed in Section 4.3.

The use of statistical data is a key issue in the data handling at the regional scale. It is employed in two ways:

- The statistical information is utilised for generation of a number of realistic crop rotations, producing the crop cover actually observed, and utilising the fertilisers consumed and the manure produced within the catchment. The amount of land under different rotations has to fit the distribution of farm types, taking into account that some types of rotations are typical for a cattle farm, others for mixed farms or for pure plant growing farms. Furthermore, the fertilisation schemes were derived for each crop based on whether the farm type produced manure, and what amounts were usually applied to the crop in question. The statistical information is thus disaggregated to produce an “intelligent” guess of the most likely distribution of factors in the study area.
- Certain parameters are highly variable, and to obtain an estimate of the effect of their variations, it is possible to conduct sensitivity analysis or Monte Carlo simulations. A sensitivity analysis provides an estimate of the uncertainties caused by a single parameter, while a Monte Carlo simulation provides an estimate of the uncertainty provided by random variations in different parameters at the same time. A sensitivity analysis can be used for pinpointing the most important parameters to be included in a Monte Carlo simulation The simulation results become an interval or a band rather than a single value. At the regional scale Monte Carlo simulations are exemplified in Section 4.4.

While upscaling receives attention in literature, the process of going from a coarser grid system in a regional model to a fine grid system in a local model is seldom considered. In practice, a local model, perhaps with very detailed local information regarding agricultural input, suffers from strong effects of boundary conditions. One approach to handle this is to let a regional model provide the boundary conditions to the local model. While this approach is considered superior to simple estimates, it has not yet been possible to quantify the derived uncertainties with respect to solute transport. However, the approach has been successfully used in hydrological studies (Refsgaard et al., 1994a and b).

4 Experiences of Non-point Pollution Simulations at Different Scales.

4.1 Performance at Point Scale

The first issue to consider is the validity of the model on the plot scale. This is important, not least to document that the process descriptions included in the model code are adequate. However, it is not always possible to obtain a full set of local data at plot scale and one may have to rely on a rougher calibration and results of preceding model validation exercises. One example of a DAISY validation exercise is shown in
*Figure **3***.

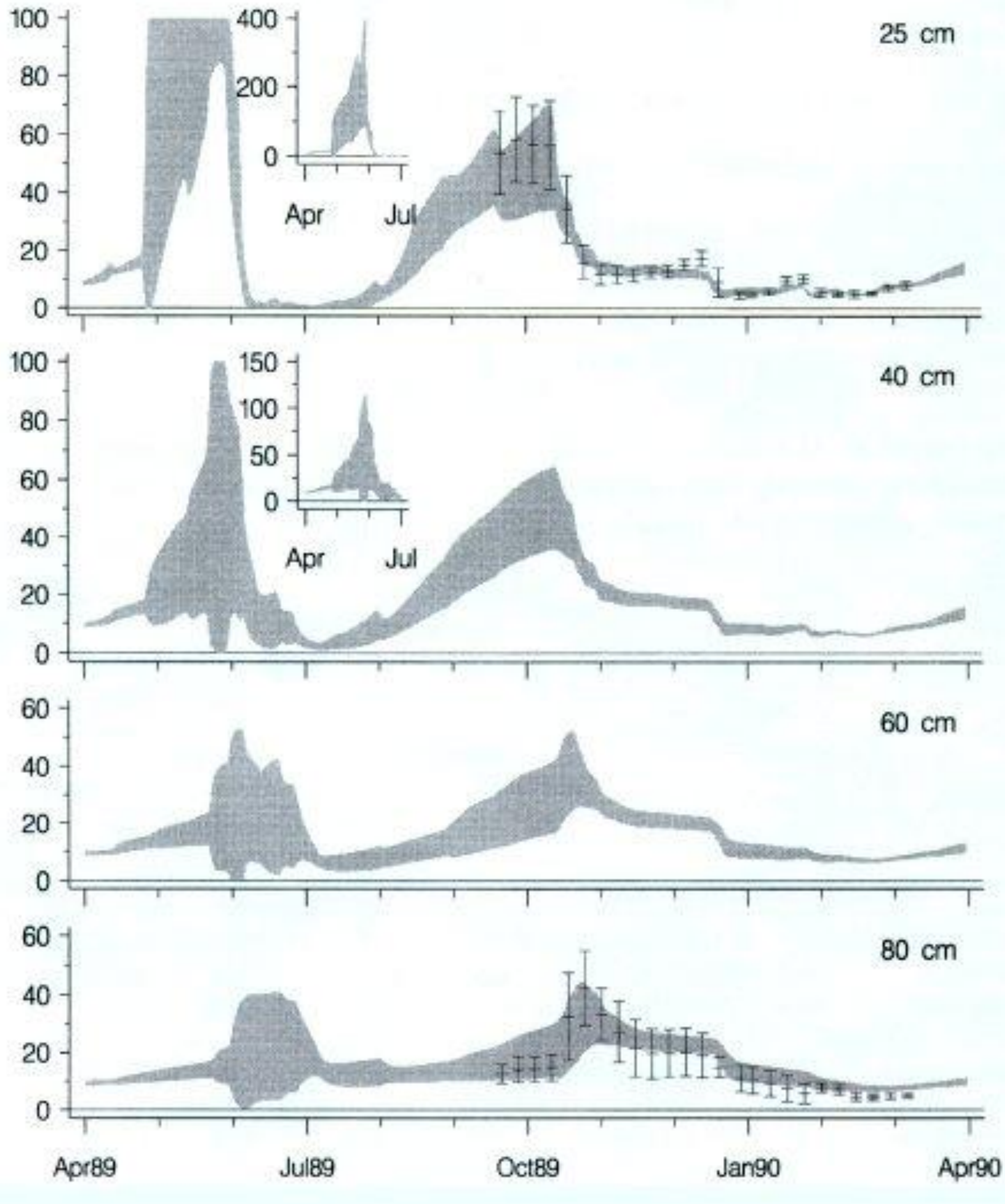


Figure 3. Simulated and measured concentrations of NO3-N (mg/l) (y-axis) at 57 points on a Jyndevad soil. Djurhuus et al. (1999) p. 272. Copyright (1999), with permission from Elsevier Science.

The figure shows the distribution of nitrate concentration measured for 57 points, compared with the distribution of 57 simulations based on locally measured parameters from the same 57 points in the field. Thus, two distributions are compared, rather than only the variation on model results compared to one set of field measurements. The correspondence between the two is impressive. As mentioned in Section 3, a substantial amount of literature documents DAISY's performance.

For pesticides, the adequacy of the simulations is less well established. DHI has been involved in a few studies concerned with evaluation of this topic for Danish conditions (e.g. Styczen and Villholth (1994). The most recent study is an evaluation of MIKE SHE SD performance for simulating one-dimensional pesticide leaching from lysimeters (Jørgensen et al., 1998).

Within the most recent project, the performance of MIKE SHE SD was compared to three widely used pesticide leaching models, PELMO (Klein, 1995), PESTLA (Boesten, 1993) and MACRO (Jarvis, 1994). Simulation of lysimeter data was conducted in two steps. First, a blind simulation without any calibration allowed was carried out and second, water and conservative solute transport processes were calibrated using measured outflow of water and bromide. No calibration of laboratory determined pesticide parameters in terms of linear sorption coefficients (K_d) and degradation half-life times ($T_{½}$) was allowed during these steps. Simulation results were evaluated using statistical tests and the outcome of these were compared to pre-determined performance criteria suggested by a European workgroup on regulatory use of pesticide leaching models (FOCUS, 1995). Further details on data background, statistical test procedures, model development, and model performance are available in Jørgensen et al. 1998 and Thorsen et al. 1998. Key results from the statistical evaluation are shown in *Table 1*.

Table 1. Results of the model performance test for simulation of Mecoprop leaching from lysimeters. The blind simulations show model performance using measured parameters without any calibration. The calibrated simulations show model performance after calibration of water and Bromide transport. No calibration on pesticide parameters was allowed in these two steps. Shadings indicate the step, if any, in which the selected performance criterion was met. A "÷" indicates that the factor-of-F test was not successful in any step.

Data type:		Accumulated percolation	Accumulated MCPP leaching	MCPP peak concentration
Statistical test:		% deviation	Factor-of-F test[1]	Factor-of-F test[1]
Performance criteria:		8 %	F = 2	F = 2
PELMO	Blind simulation	10	÷	÷
	Calibrated	10	÷	÷
PESTLA	Blind simulation	13	÷	÷
	Calibrated	6	÷	÷
MACRO	Blind simulation	8	F = 2	F = 2
	Calibrated	2	F = 2	F = 2
MIKE SHE	Blind simulation	12	F = 2	F = 2
	Calibrated	7	F = 5	F = 2

[1] The factor-of-F test compare simulated values with the range of measured values from the 2 lysimeters. F = 2 or F = 5 indicate that simulation results lie within a factor of 2 or 5, respectively, from the measured values. The statistical tests are further described in Jørgensen et al. (1998) and Thorsen et al. (1998). MCPP: Mecoprop.

The experimental data showed that water flow and pesticide leaching was primarily controlled by preferential flow through a small active pore volume. The main results of the model performance test was that the two model codes containing a description of preferential flow (MACRO and MIKE SHE) passed the performance criteria for pesticide flux already in the blind simulation whereas PELMO and PESTLA required calibration which violated the original parameterisation (results not shown).

4.2 Modelling at Local and Catchment Scale

Several studies contain the approach of moving from plot scale to small catchment or regional scale. *Table 2* contains a sample of studies conducted with DHI involvement showing the area simulated, the resolution used, and the data sources.

Table 2. Overview of scale, resolution and data sources used in different studies presented.

	Scale	**Grid size**	**Data**
NPo-project-Karup			
Experimental plots	plot size	plot size	Local
Rabis Creek	16 km^2	400 m	Local and Regional/ statistical
Karup Stream catchment	440 km^2 (groundwater catchment)	500 m	Regional/ statistical
Pesticides in groundwater			
Karup Stream catchment	440 km^2 (groundwater catchment)	1 km	Regional/statistical
Fladerne Creek	4 km^2	100 m	Local
Vaarby Stream	360 km^2	1 km	Regional/statistical
Lungrende Creek	4 km^2	100 m	Local
Pesticide in surface water			
Intensively monitored fields	plot size	plot size	Local
Lillebæk catchment	4.7 km^2	Not yet determined, approx. 25 m	Data for each field. Some data will be treated statistically.
Brøns creek			
local scale	10 km^2	Not yet determined, approx. 50 m	Local
regional scale	100 km^2	Not yet determined, approx. 200 m	Regional/statistical
UNCERSDSS*			
Karup Stream catchment	518 km^2 (topographic catchment)	1, 2, 4 km	EU-scale
Odense Stream catchment	536 km^2	1, 2, 4 km	EU-scale

*UNCERSDSS: Uncertainty of spatial decision support systems, EU reseach project.

4.2.1 The Karup study

The first study, which was conducted with MIKE SHE/DAISY, took place in the Karup catchment in Jutland (Storm et al., 1990; Styczen and Storm 1993a and b). In practice, simulations took place at three scales, as shown in *Table 2*. The physical location of the Karup catchment is shown in *Figure 4*.

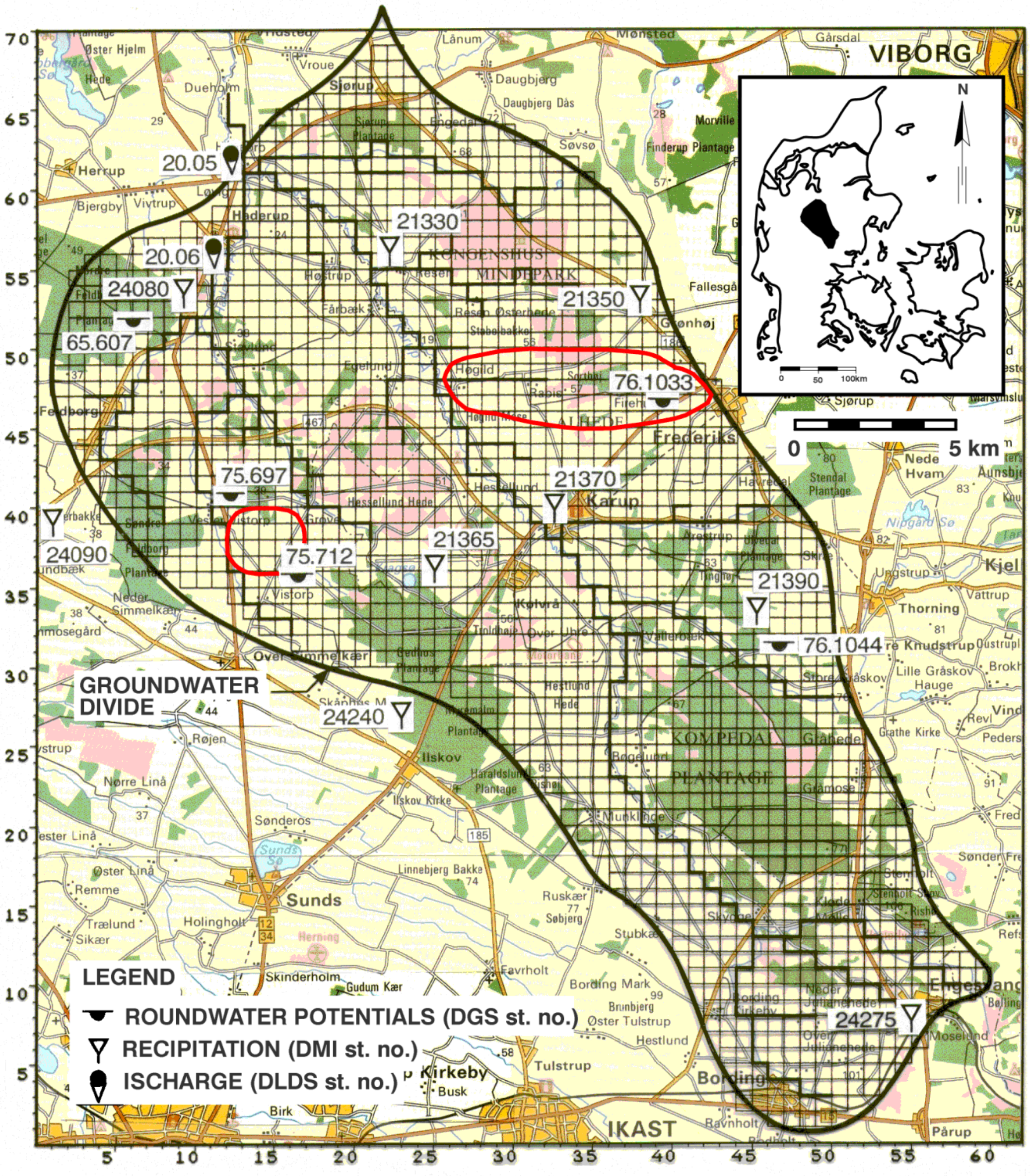


Figure 4 The Karup groundwater catchment. The catchments for Rabis Creek and Fladerne Creek, also mentioned in the text, are indicated with red, Rabis creek towards the east and Fladerne creek to the west.

The plot scale simulations were carried out by DHI as part of the initial work of setting up the regional model, but were never published. For Rabis Creek, detailed simulations of water flow, and tritium movement were carried out, together with some geochemical modelling of nitrate, mainly concerned with processes taking place along the redox front by Engesgaard and Jensen (1990).

The regional model is based on the results from the plot simulations and the detailed study of Rabis Creek. Furthermore, it is based on data from local meteorological stations, all available map information (soils, topography, land use), statistics on fertiliser use, number of animals, and farm types, interviews with agricultural consultants, interpreted geological profiles and geological data from boreholes, stream flow data, and groundwater head, monitored during part of the simulation period.

The data interpretation included, among others, positioning of permanent grass areas in areas with shallow groundwater identified through preliminary simulations with MIKE SHE. The agricultural data were interpreted as described in Section 3. Similarly, the tillage methods chosen and the methods of manure storage assumed changed over the simulation period according to the information given and the crop simulated. Land use and the distribution of crop rotations are shown in *Figure 5*. The redox front was interpolated from information from the 120 boreholes.

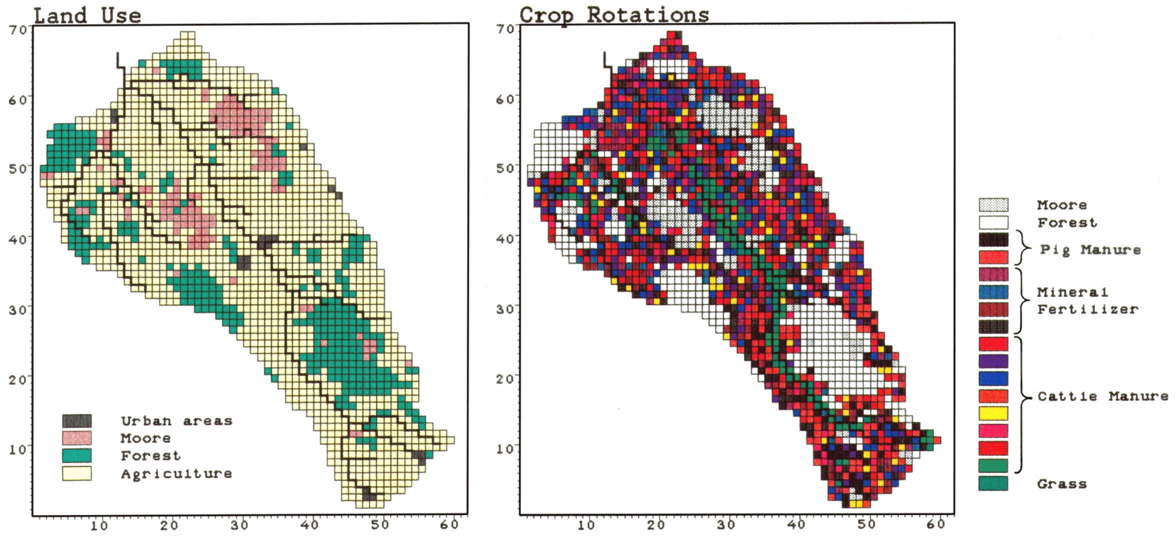


Figure 5 Distribution of crop rotations in the Karup catchment.

To test the adequacy of the regional model, the Rabis Creek subcatchment was simulated with smaller grids, and the results were compared to actual measurements in the groundwater. As the data in the regional model was based on statistics, the results could not be expected to be correct in a given point. Two simulations were carried out: a) with the statistical input, and b) with the average of the statistical input for all cells. The data sources and in the latter case, the treatment are identical for Rabis Creek and the Karup catchment and the grid resolution is almost identical. The simulated result and the observations showed a large degree of accordance, when the discretisation of the saturated zone was taken into account. Features such as effects of rather wet or dry years clearly showed up in the results. The distribution of nitrate in time and space is documented in Storm et al. (1990) and Styczen and Storm

(1993b). With good results in Rabis Creek, it was expected that the regional simulations would be adequate, as the grid size was almost unchanged, and the database was identical. Only the size of the area differed. An example of the output is shown in *Figure 6*.

While the overall flow parameters of Karup were simulated very well for the catchment the simulated nitrate concentrations in the river were much larger than the observed. The plausible reason for this is the high denitrification, which takes place in the wetland areas near Karup Stream. This process was not included in the model at the time.

A similar analysis was later carried out for Danube Island in Slovakia (Refsgaard et al., 1998).

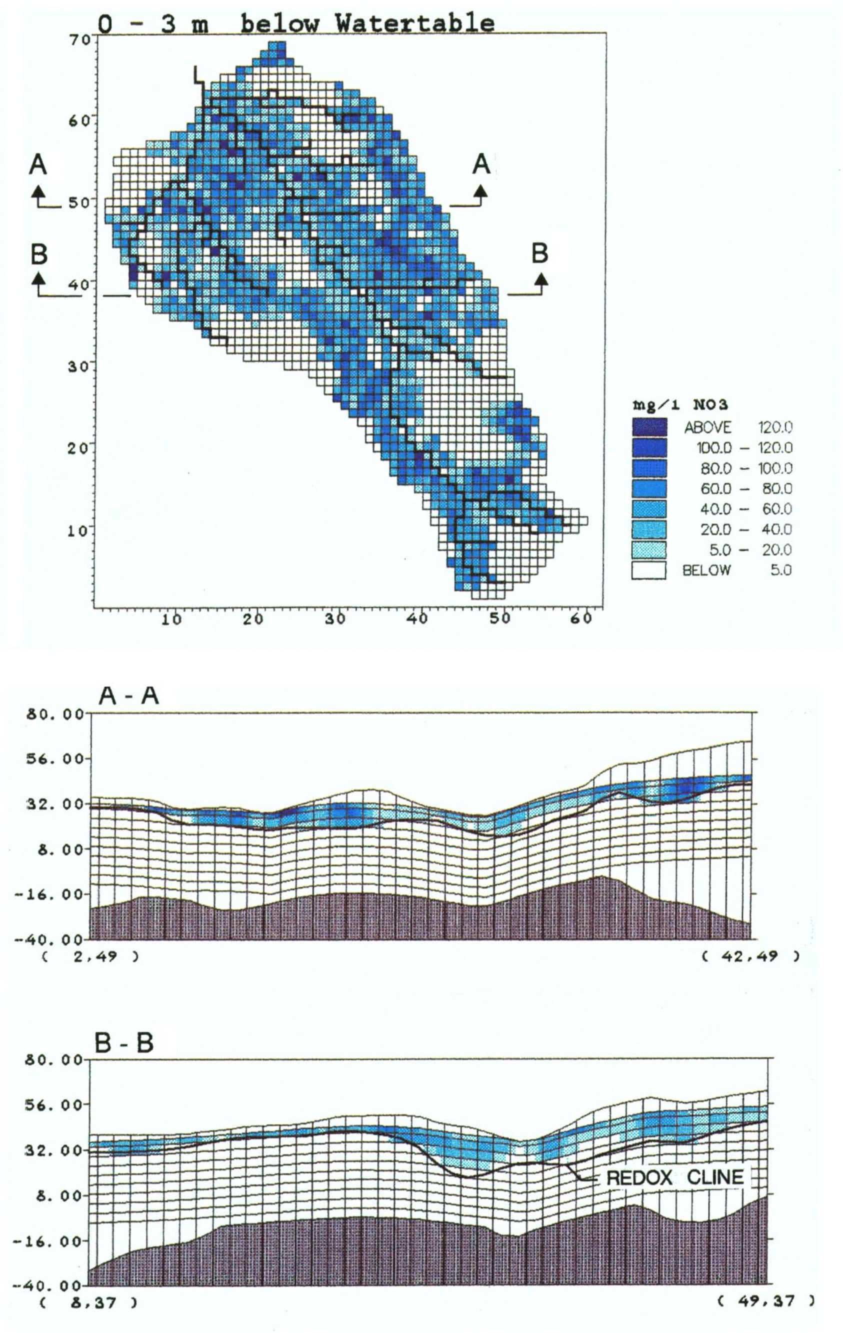


Figure 6. An example of distribution of nitrate concentrations in the groundwater of Karup catchment.

4.2.2 Pesticides and groundwater

In an ongoing project under the strategic environmental scientific program by the Danish Ministry of the Environment the scaling problem is being investigated within the frame of agricultural use of pesticides and the impact of the groundwater. Three target pesticides are in focus: Mecoprop, Bentazon, and Isoproturon. Field investigation and subsequent modelling is taking place on two different scales. In this case the scaling problem refers to the differences in the area extent and data resolution.

Two field sites have been chosen as representative for Danish conditions. The Karup catchment in the central part of Jutland and the Vaarby catchment in the western part of Zealand have been selected as representatives for large scale sandy and clayey till (overlain by sandy loam) soils, respectively. Within these two catchments two sub catchments (the Fladerne catchment in Jutland and the Lungrende catchment at Zealand) have been selected to reflect the small catchment scale. The area extent of the catchments is shown in *Table 2* and the location of Fladerne Creek in *Figure 4*.

The pesticide input function and the validation of the models depend on the scale. In the case of the two small catchments, interviews have been conducted with the local farmers and their consultants to map the use of crop specific pesticides during the last few years in detail. Also, monitoring of the pesticide content in the groundwater and in the stream discharge is being performed to enable validation.

A similar procedure with interviews is not possible at large scale. Hence, the pesticide input function is created by the use of agricultural statistics of the general crop use and crop specific pesticides during the last decade in the area. A similar line of approach was used in the NPo-project (Section 4.2.1) with respect to the agricultural use of fertiliser. No monitoring of the pesticide content in the groundwater and in the stream discharge is being performed.

Preliminary results from laboratory investigations have indicated that microbial degradation takes place in the aerobic zone of the hydrological system. However, the target pesticides persist when oxygen is not present. Also, it is shown that the pesticide sorption among others depends on the concentration of pesticides. Laboratory experiments have indicated that the three target pesticides do not behave identically with respect to process description and parameterisation. Thus, the application of an advanced model for transport and metabolism seems to be of importance.

4.2.3 Pesticides in surface water

The objective of this project is to produce a tool for evaluation of pesticide in surface water, to be used by the Danish Environmental Protection Agency, in connection with pesticide registration.

In this project, which is still in its initial phase regarding modelling, pesticide will be simulated on plot scale and in a small catchment of 4.7 km^2. A detailed monitoring programme for 6 experimental plots, on which all input is known (pesticides, fertiliser, manure, tillage, etc) provides validation data. Moisture, drain flow, groundwater level, nitrate in soil moisture and nitrate and phosphorus in drain flow and groundwater are being observed frequently. Pesticide is also monitored in connection with some of the plots. The information from the plots will be utilised for calibration of water flow and nitrate-related processes (inclusive of solute transport). Phosphorus will be used as an indicator for colloid transport in macropores and drains, which also takes place with respect to pesticides.

For the small catchment, detailed information will be available concerning crops and spraying practices on all fields. Pesticides are monitored in drains and in the stream. In this case, the data related to agricultural input exists almost as detailed for the entire area as for the plots. However, the soil information available and of course the calibration/validation data are found on a larger scale. The resolution of the final setup is expected to be below field size (i.e. 25x25 m).

Regarding transport pathways, the study is most comprehensive, as drift, macropore flow, colloid transport and soil erosion are considered, on top of the usual pathways. This project may be followed on http://projects.dhi.dk/pesticide.

4.2.4 Brøns Creek – Generating boundary conditions to a local model

DHI has used regional hydrological models as boundary conditions for more detailed models for some time. Regarding solute transport, however, it is a new approach. In a recently started project in Brøns Creek the approach will be tried out.

A river restoration project for a small section of the Brøns creek in the Southern part of Jutland, Denmark, has been initiated. The section is about 5 km long with a topographical catchment area of approximately 10 km^2. It is the lower part of a hundred-km^2 river catchment mainly covered with farmland and plantation. The project goal is to increase the potential for NO_3 removal in the wetland areas along the creek.

Measures to increase the denitrification processes include restoration of the old creek course water level rise in the creek by “semi-natural” submerged weirs, and cutting off all artificial drainage pipes and ditches in the catchment. It is planned to apply the models mentioned earlier on different scales to demonstrate the possible effect of the restoration project.

On the 10 km^2 scale (local scale) it is possible to obtain detailed information on land-use for each field in the catchment for the last five years both with respect to crop type and fertiliser type and amount. This information forms the main input to MIKE SHE DAISY.

It has been decided to construct a model covering the entire one hundred-km^2 catchment (regional scale) for two reasons:

1. To generate realistic, time-varying boundary conditions to the local scale model in terms of water and NO_3 fluxes and groundwater head variations,
2. To allow calibration of the model on measured discharges and NO_3 fluxes in a gauging station located at the outlet of the local (and regional) scale area.

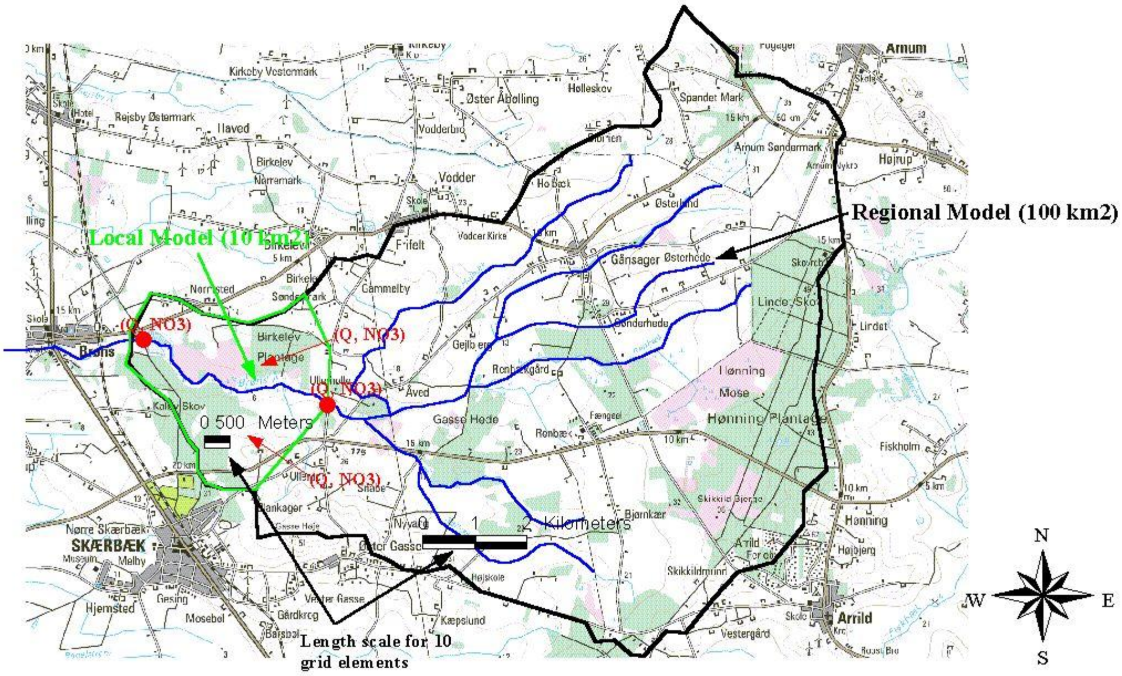


Figure 7. The regional (black boundary) and local (green boundary) catchments for Brøns Creek. The resolution is tentatively assumed to be 50 and 200 m for the local and regional model, respectively. The two scales on the figure thus indicates the length of 10 grids for each of the two models.

For the larger area it is impossible to obtain deterministic values of land-use and fertiliser application and the statistical approach was applied to allow DAISY to generate infiltration of water and NO_3 to MIKE SHE. Firstly, the area will be divided into main land use types – farmland, plantation, urban areas and areas with permanent grass. Secondly, the statistics and the agricultural information available will be used to define sets of crop rotations and cropping practices, which will be distributed randomly over the farmland, as explained in Section 3 and 4.2.1. A simple approach for NO_3 degradation in the groundwater zone was introduced similarly to the approach used in the Karup study (4.2.1).

The regional simulation will be used to generate the boundary conditions in the form of water and solute fluxes for local scale modelling.

4.3 Effects of Grid Resolution

The smallest horizontal discretization in a distributed model is the grid size, which is typically larger than the field scale at which parameters are determined. Running the model at large grid resolutions but using model parameters valid at field scale is necessary to make the computational demand acceptable for large catchments or regional scale applications. A critical question is, therefore, how the catchment scale model output is influenced by selection of grid resolution. The following comparisons concern grid sizes of 1, 2 and 4 km^2.

Two study areas were included in the analysis: the Karup stream catchment and the Odense stream catchment. The main differences between these two catchments are that where the Karup catchment is characterised by flat topography, coarse topsoil texture, and rather uncomplicated geology with unconfined conditions in the aquifer, the Odense catchment has a more varied topography, topsoils belonging to more fine textured classes, and more complex geology with confined groundwater conditions. The catchment characteristics, data background, and model construction are further described in UNCERSDSS (1998) and Refsgaard et al. (1999). An important difference to the earlier Karup study is that data, where possible, was obtained from European data bases which influenced the model construction. For example, the topographic catchment rather than the groundwater catchment was delineated and the geological description was considerably simplified.

Most spatial data from the EU-databases were obtained in 1-km grid resolution and the initial model construction therefore corresponded to this. The grid up-scaling was partly done automatically by the MIKE SHE model set-up-program, which uses the basic data files to establish a model with a larger user-specified grid resolution. However, manual adjustments were necessary in order to secure that the topographic representation matched the location of the river network while changing grid resolution and that the location of crop rotations matched the location of land use types.

Key results from simulations with different grid resolution are shown in *Table 3* and *Table 4*, and in *Figure 8*. The results show that the simulated annual runoff is almost identical and thus independent of grid sizes. An explanation of the minor differences is that the catchment areas in the 1, 2 and 4 km models were not exactly identical. Thus, the root zone processes responsible for generating the evapotranspiration and consequently the runoff do not appear to be scale dependent as long as the statistical properties of the soil and vegetation types are preserved, which is the case with the applied aggregation procedure.

Table 3. Key results from simulation of the Karup catchment (518 km^2) with varying grid resolution (1, 2 and 4 km). Averaged results over the five-year period 1989-1993. Average annual precipitation was 884-mm $year^{-1}$.

	1 km	2 km	4 km	Observed
River flow (mm $year^{-1}$)	460	461	444	451
% of area > 50 mg NO_3 l^{-1}	50.4	55.5	51.6	57
Av. Conc. (mg NO_3 l^{-1})	45.5	47.2	47.3	58

Table 4 Key results from simulation of the Odense catchment (536 km^2) with varying grid resolution (1, 2, and 4-km). Averaged results over the five-year period 1989-1993. Average annual precipitation was 805-mm $year^{-1}$.

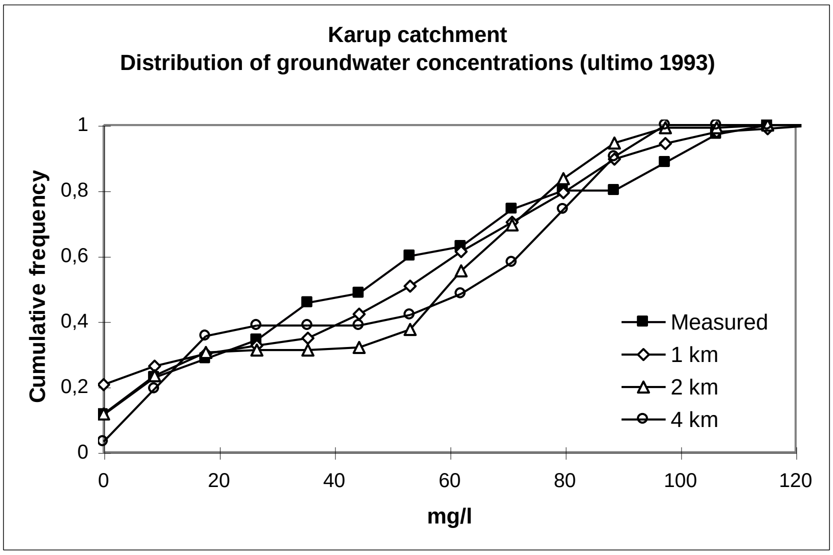
	1 km	2 km	4 km	Observed
River flow (mm $year^{-1}$)	305	291	315	259
% of area > 50 mg NO_3 l^{-1}	9.5	4.8	4.25	0
Av. Conc. (mg NO_3 l^{-1})	24.5	17.9	15.3	2

The hydrograph shape differed significantly for the three grid sizes (not shown). For the Karup model, the simulation with 1 km grid reproduced the low flow conditions reasonably well, whereas the 2 and 4 km grids had a rather poor description of the baseflow recession in general and the low flow conditions in particular. For the Odense model, the simulation with the 1 km grid showed too large baseflows during the low flow season, while the 2 km grid model obtained an appropriate level and the 4 km grid model simulated less low flow than observed. This indicates that there are significant effects of grid size on the stream-aquifer interaction that are not properly described in the applied aggregation procedure.

The simulated nitrate concentrations in the groundwater differ considerably between the two catchments. Higher average concentrations are simulated in the Karup catchments compared to the Odense catchment (*Table 3* and *Table 4*). For the Karup catchment the simulated nitrate distributions (*Figure 8*) compare rather well with measured data in terms of both shape and level. For the Odense catchment the simulated distribution of nitrate concentrations do not compare very well with the measured data. 80 % of the observation wells of the Odense catchment showed no nitrate whereas the model simulated zero concentration in only 25 % of the area. Thus, the simulated nitrate concentrations in the groundwater were not clearly influenced by the grid size for the Karup catchment, while there appeared to be some effect for the Odense catchment.

The explanation of these differences is found to the different hydro-geological situations in the two catchments. In the Karup catchment the groundwater table is generally located a couple of meters below terrain surface and the horizontal flows take place in both the Quaternary and the Miocene sediments. Hence, independent of grid resolution, the main part of the horizontal groundwater flow takes place in the about 15 m of the aquifer located above the reduction front. Only a relatively small part of the flow lines cross the reduction front, below which, the nitrate is assumed to disappear. In the Odense catchment, the horizontal groundwater flows take place almost exclusively in the lower aquifer, of which only the upper 3 metres are located above the reduction front. This implies that a large part of the groundwater flow is crossing the reduction front on its route from the infiltration zones in the hilly areas towards the discharge zones near the river. As the size of the grid influences the smoothness of the aquifer geometry, the grid size will significantly influence the number of flow lines crossing the reduction front and hence the nitrate concentrations. This scaling effect of the hydro-geological conditions is not accounted for in the present aggregation procedure.

It is noticed that the nitrate concentrations are significantly lower in the Odense catchment compared to the Karup catchment, with respect to both the observed and the simulated values. The main reason for this is that the different soil properties and the smaller number of animals result in a lower nitrate leaching from the root zone in the Odense catchment.



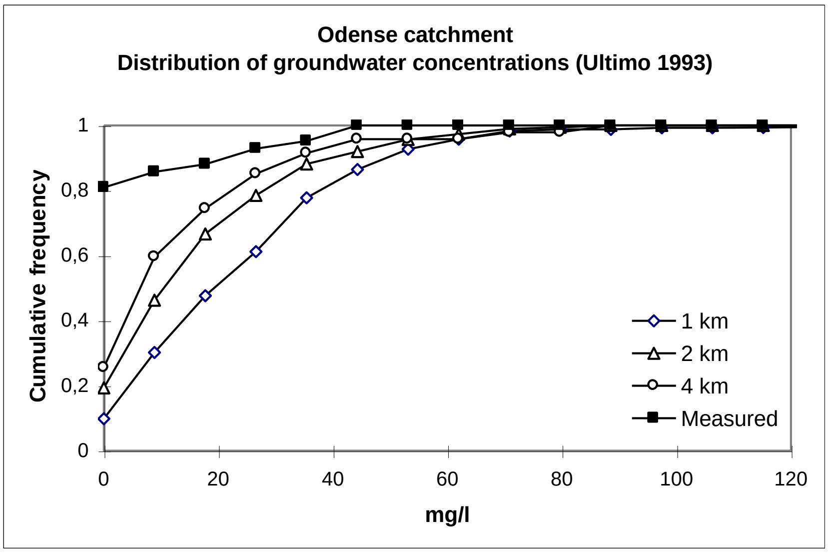


Figure 8 Measured and simulated distributions of nitrate concentrations in upper groundwater in the Karup and the Odense stream catchments at the end of the simulation period. Measured distributions are based on 35 obervations in the Karup catchment and 42 observations in the Odense catchment.

4.4 Uncertainty of Input Data

A simple way to compare effects of input data would be to simulate the same area based on two different datasets, generated from different sources. As may be seen from *Table 2*, the Karup catchment has been simulated with different data sources, but unfortunately not for the same period of time. The hydrology of the Odense catchment has been simulated twice: a) by applying local data (the client being the County of Funen) or b) with data from the EU-databases (in an EU-project). It is evident that the local data produce much more convincing results compared to the use of EU-databases as data source. A primary explanation of this discrepancy is the much better geological description obtained with local data.

Effects of input uncertainty may be judged through Monte Carlo simulations.
In the above-mentioned EU project, the uncertainty in simulated nitrate concentrations in groundwater aquifers was estimated using European level data sources readily available from standard European databases such as GISCO and EUROSTAT as the basis of the modelling. Where crucial data were found missing these were obtained from readily available national data sources. The model parameters were all assessed from these data by use of various transfer functions and no model calibration was carried out. Furthermore, a statistically based aggregation procedure, preserving the spatial distribution of soil types, vegetation types, etc. on a catchment basis was adopted.

The study area used for the uncertainty analysis was the Karup catchment, which is further described in Styczen and Storm (1993a,b). The data used for the study and the model construction are described in details in UNCERSDSS (1998), Refsgaard et al. (1999) and Hansen et al. (1999). The grid resolution used for the uncertainty analysis was 2 km. In the simulations, the DAISY model produced calculations of water and nitrogen behaviour from soil surface and through the root zone acting as source input to the MIKE SHE grids, which were allocated to agriculture. In the grids allocated to natural areas, MIKE SHE calculated the water percolation whereas no nitrate contribution was assumed from these areas. As the integration between DAISY and MIKE SHE was not made at code level when this project was conducted (*Figure 1*), feedback from MIKE SHE to DAISY through fluctuating groundwater was not considered. A seven-year period was simulated (1987-1993) of which the two first years were used for model warm-up.

Uncertainty analyses were performed using Monte Carlo technique where the deterministic model was run several times using different (equally probable) realisations of the input/parameter field. Ideally, all model parameters should be included in the uncertainty analysis. However, the MIKE SHE DAISY modelling system contain a very large number of input parameters, which, if all were to be treated stochastically, would require an unrealistic number of Monte Carlo simulations and CPU-time. Thus, a selection of only five types of model parameters was made using expert judgement to evaluate the expected relative influence of different model parameters on the type of model results, which were of particular interest in the present study, namely the nitrate concentrations of the aquifer. The magnitude of the error associated with each of the five stochastic parameters was, if possible, determined on the basis of information on the uncertainty related to the data source. If no information existed, the magnitude of the uncertainty was estimated by expert judgement. After evaluation of a number of test simulations, a total of 25 Monte Carlo runs were found adequate for the uncertainty analysis. The five stochastic parameters were

- Daily precipitation amount. The constraints were to keep dry days dry and to normalise series in order to preserve the mean value over the 25 Monte Carlo runs.
- Soil hydraulic properties determined by pedo-transfer functions based on soil textural composition. The clay content within each texture class of the GISCO soil map was treated stochastically.
- Slurry composition
- Soil organic matter content.
- Location of nitrate reduction front in the aquifer.

Most of the stochastic parameters were related to the DAISY model. DAISY was not run in each grid cell in the catchment but only for each of 17 crop rotation types in order to limit the CPU time consumption. Thus, the stochastic parameters were not treated as spatially varying, but rather as spatially constant values. All stochastic parameters were treated as being mutually independent (uncorrelated). The reason for this was that the information for estimating correlation between the stochastic parameters was lacking and that no high degree of correlation was suspected a priori.

The key results from the Monte Carlo runs are shown in *Table 5*. The results are averaged over the five-year output period and the mean and standard deviations represent statistical values from the 25 Monte Carlo runs. The uncertainties on the simulated average groundwater concentrations are further shown in *Figure 9*.

Table 5 Key results from 25 Monte Carlo runs. Simulation results are averaged for the entire catchment area and over the 5 year simulation period.

Variable	Mean	St.dev.	CV* (%)
Leaching from the root zone (kg ha^{-1} $year^{-1}$)	65	19	29
Groundwater concentration (mg l^{-1})	48	8	17
River flow (mm $year^{-1}$)	464	22	5

* Coefficient of variation

Generally, less uncertainty was associated with the water balance component and river flow (CV=5 %) than to the components of the nitrogen balance i.e. nitrate leaching (CV=29 %) and nitrate concentrations in groundwater (CV=17 %) (*Table 5*). The uncertainty of simulated river flow was dominated by contributions from uncertainty on soil texture (influencing soil hydraulic parameters) and of precipitation, whereas the uncertainties associated with components of the nitrogen balance were dominated by the uncertainty contributions from both soil texture, soil organic matter and slurry composition.

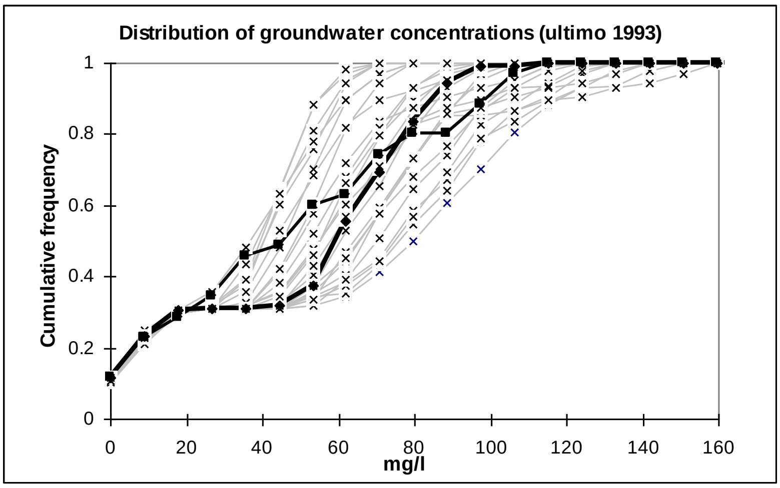


Figure 9 Statistical distribution of groundwater nitrate concentrations in the Karup catchment by the end of the simulation period. . X = Simulated Monte Carlo distributions (25), ● = Deterministic simulation using 'best guess' parameters, ■ = measured distribution based on 35 groundwater boreholes.

Uncertainty of precipitation contributed only to a minor degree to the simulated uncertainties of the nitrogen components despite the influence it had on the water balance. The depth of the reduction front appeared to have only minor influence on the uncertainty on stream water concentrations in the present simulations.

The case study indicates that, for the Karup catchment, the uncertainty of the predicted nitrate concentrations in the aquifer at a scale of some hundreds of km^2 is so relatively small that the methodology appears suitable for large scale policy studies. Results also show that even though the uncertainty of the simulated results is large at point/field scale, making the predictive capabilities questionable, it appears that the uncertainty at larger scales, where the point simulations are integrated in time and space, decrease considerably, making the simulation results appear more useful. Given the rather coarse data basis and given that no model calibration was performed, the simulated results of groundwater concentrations were remarkably good. Hence, the measured groundwater concentrations fell well within the predicted uncertainty intervals. As the Karup catchment is characterised as having flat topography and rather simple geology, it is most likely that the obtained results may differ for a catchment with a more varied topography and complex geology (see also Section 4.3).

5 Discussion and Conclusions

For simulation of water and nitrate, the models used have proven their worth at plot or field scale. It is therefore not surprising that it is possible to scale up area-wise, using the same, or almost the same grid resolution and level of detail in the data. A major leap occurs, when moving from “real” to statistical data. The experience from the different studies with nitrate simulations has been that this leap is indeed possible. However, a critical view on the evaluation of output is required. Due to the fact that the input is not geo-referenced, the comparison with output cannot be either. The model, therefore, cannot reproduce the concentration at a specific location in the catchment. It can represent the statistical distribution of concentrations in a given layer. Integrated outputs such as streamflow can also be simulated through the statistical approach.

It is interesting to notice that the distributed input (although based on statistics) is a requirement for a realistic result. In the UNCERSDSS project, an attempt was made to substitute the rotation approach by simulation of the dominant crop. The results were clearly erroneous. (*Figure 10*). The distribution of concentrations in the groundwater is very much a function of the interpretation of statistical data in terms of agricultural practice. This initial data interpretation therefore requires the necessary time and expertise.

For simulation of annual runoff and nitrate concentrations, both of which are affected primarily by root zone processes, the impact of changes of grid resolution is relatively small. Contrary to this, the impact on hydrograph shape is consistently rather large. This finding, which also is documented earlier in Refsgaard (1997), indicates that the applied aggregation procedure has important limitations with respect to describing the stream-aquifer interactions. An important point is that the applied methodology is scale dependent with regard to hydrograph simulation; hence a change of grid size generates a need for recalibration of parameters responsible for baseflow recession and low flow simulation.

The Monte Carlo simulation exercise showed that it is possible to use Monte Carlo simulations to provide a good estimate of uncertainties in simulated groundwater concentrations if the basic model description is reliable. This makes simulation results more valuable for decision making.

Thus, the conclusion is that the data requirements seldom pose insurmountable problems for regional modelling, if the models used are considered reliable for the conditions to be investigated and if the aggregated results are sufficient for the decisions to be taken. For most political decision, it is the aggregated output, which are required. However, attention must be paid to the geology of the area, which is not adequately described in databases at EU level. National databases may, however, contain adequate data.

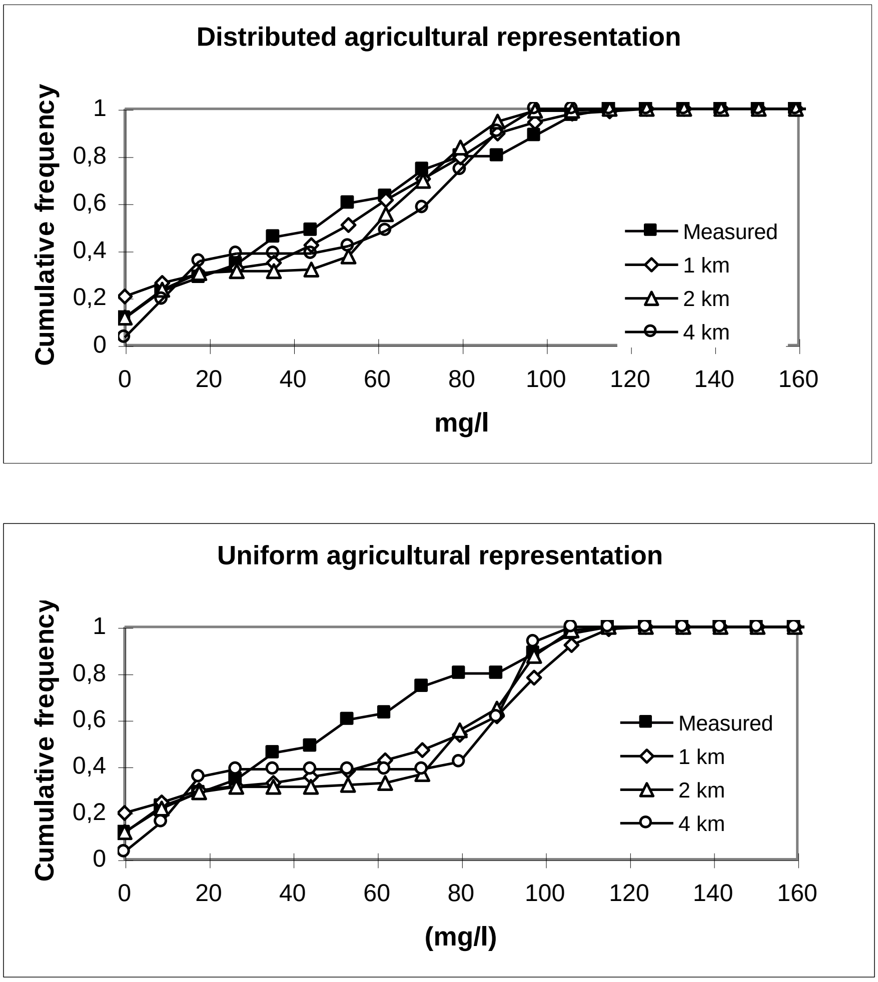


Figure 10 Observed and simulated distribution of nitrate concentrations in the groundwater at the end of the simulation period (Karup catchment).

For pesticides the picture is somewhat less clear at present. Generally, the pesticide models produce less convincing results than the other mentioned models, not least because the precision required of the simulations is very high. For comparison, the drinking water requirements state a concentration of less than 0.1 µg/l. If the pesticide application is 1 kg/ha and the application area is Eastern Denmark, it is necessary to precisely account for the last

1/5000 of the applied chemical. Heterogeneity may turn out to be of greater importance for such simulations than for e.g. nitrate. The results of the ongoing projects should indicate whether the statistical approach is valid also for this type of simulations.

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