Modelling Water Discharge and Nitrogen Loads from Drained Agricultural Land at Field and Watershed Scale

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Abstract

This thesis examines water discharge and NO_3-N loads from drained agricultural land in southern Sweden by modelling at field and watershed scale. In the first stage of the work, the ability of DRAINMOD to simulate outflow in subsurface drains and that of DRAINMOD-N II to simulate NO_3-N loads in these drains was evaluated in field experiments. In addition, the ROSETTA pedotransfer model was used to estimate soil hydraulic properties required by DRAINMOD. In the second stage, DRAINMOD was integrated with Arc Hydro in a GIS framework (Arc Hydro-DRAINMOD) to simulate the hydrological response of an artificially drained watershed. DRAINMOD-N II and a temperature-dependent NO_3-N removal equation were also included in Arc Hydro-DRAINMOD to predict NO_3-N loading. Arc Hydro-DRAINMOD used a distributed modelling approach to aggregate the results of field-scale simulations, where the Arc Hydro data model described the drainage patterns in the watershed and connected the model simulations from fields through the stream network to the watershed outlet. GLUE methodology was applied to estimate uncertainties in the framework inputs. At field scale, monthly values of drain outflows simulated by DRAINMOD and NO_3-N loads simulated by DRAINMOD-N II showed good agreement with observed values. Good agreement was also found between observed and DRAINMOD-simulated drainage rates when ROSETTA-estimated K_s values were used as inputs in DRAINMOD. At watershed scale, temporal trend and magnitude of monthly measured discharge and NO_3-N loads were well predicted by Arc Hydro-DRAINMOD, which included uncertainty estimation using GLUE methodology. Sensitivity analysis showed that NO_3-N loads from the stream baseflow and N removal in the stream network processes had the most sensitive parameters. These results demonstrate the potential of DRAINMOD/DRAINMOD-N II and Arc Hydro-DRAINMOD for simulating hydrological and N processes in drained agricultural land at field and watershed scale. These models can contribute to improve water use efficiency in watersheds and to evaluate best management practices for preventing surface water and groundwater pollution.

Keywords: Arc Hydro, controlled drainage, DRAINMOD, GIS, GLUE, ROSETTA

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To my sons Emilio and Alejandro
and my wife Ariela

The most incomprehensible thing about the world is that it is at all comprehensible.
Albert Einstein

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List of Publications

This thesis is based on the work contained in the following papers, which are referred to in the text by their Roman numerals:

I Salazar, O., Wesström, I. & Joel, A. (2008). Evaluation of DRAINMOD using saturated hydraulic conductivity estimated by a pedotransfer function model. *Agricultural Water Management* 95(10), 1135-1143.

II Salazar, O., Wesström, I., Youssef, M.A., Skaggs, R.W. & Joel, A. (2009). Evaluation of the DRAINMOD–N II model for predicting nitrogen losses in a loamy sand under cultivation in south-east Sweden. *Agricultural Water Management* 96(2), 267-281.

III Salazar, O., Joel, A., Wesström, I., Linnér, H. & Skaggs, R.W. Modelling discharge from a coastal watershed in south-east Sweden using an integrated framework (submitted).

IV Salazar, O., Wesström, I., Joel, A. & Youssef, M.A. Application of an integrated framework for predicting nitrate loads from a coastal watershed in south-east Sweden (submitted).

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The contribution of Osvaldo Salazar to the papers included in this thesis was as follows:

I Performed data analysis, simulations and writing, with assistance from the co-authors.

II Performed data analysis with assistance from Dr. Wesström, simulations with assistance from Dr. Skaggs and Dr. Youssef, and writing with assistance from the co-authors.

III Performed framework development and simulations with assistance from Dr. Joel, and writing with assistance from the co-authors.

IV Performed framework application with assistance from Dr. Wesström, and writing with assistance from the co-authors.

Abbreviations

ANN	Artificial neural network
BMPs	Best management practices
CD	Conventional drainage
CWT	Controlled drainage
d	Index of agreement
$d_{K\text{-}S}$	Kolmogorov-Smirnov *d* statistic
DEM	Digital elevation model
E	Modelling efficiency
E_d	Accumulated deviation
ET	Evapotranspiration
F	Infiltration
GIS	Geographical information system
GLUE	Generalised Likelihood Uncertainty Estimation
LK_s	Lateral saturated hydraulic conductivity
K_s	Vertical saturated hydraulic conductivity
MAE	Mean absolute error
MC	Monte Carlo simulation
NO_3–N	Nitrate-nitrogen
PTFs	Pedotransfer functions
SA	Sensitivity analysis
UA	Uncertainty analysis

1 Introduction

The loss of nutrients from agricultural land is a major non-point source pollution to surface waters and groundwater in many regions (Oenema *et al.*, 1998; Hooda *et al.*, 2000; Randall & Mulla, 2001; Stoate *et al.*, 2001). Intensive use of fertilisers and manure to aid food production has increased nitrogen (N) and phosphorus (P) levels in surface water bodies, promoting eutrophication and stimulation of algal growth (Schindler, 1990; Carpenter *et al.*, 1998).

In Sweden, diffuse nutrient losses from agricultural land became more important than point sources after the improvement of Swedish municipal and industrial waste water treatment three decades ago (Ulén & Fölster, 2007). Drained land under intensified fertilisation may have led to an increase in the N load on Swedish coastal ecosystems (Larsson *et al.*, 1985; Krug, 1993). For instance, Andersson & Arheimer (2003) modelling nitrogen (N) loads in a Swedish river during 1885-1994 found that land drainage had an important impact on the decline in soil N retention, which increased the N loads. One major concern is coastal areas of southern Sweden, which are more prone to N leaching because they have coarse-textured soils with low water-holding capacity, where N transport in lowland rivers has resulted in serious coastal eutrophication problems (Larsson *et al.*, 1985; Stålnacke *et al.*, 1999). This ongoing eutrophication has led to widespread hypoxia in bottom areas in marine coastal ecosystems in southern Sweden (Vahtera *et al.*, 2007).

The mechanisms determining the hydrology and loss of N from artificially drained soils are complex and depend on many factors, such as land use, management practices, soil type, site conditions and climate (Skaggs *et al.*, 1994). The development of hydrological models has allowed the mechanisms of N retention and release in these drained areas to be described (Thomas *et al.*, 1992). Quinn (2004) noted that the role of models in reflecting our understanding of nitrate losses is important for the final establishment of best management practices (BMPs) in nitrate management.

One of the most widely applied hydrological models is DRAINMOD (Skaggs, 1978, 1999). The current DRAINMOD-N II version 6.0 (Youssef *et al.*, 2005) includes a module for simulating N and carbon dynamics that is based on the water balance calculations of the standard DRAINMOD. Soil hydraulic properties are needed as input variables to run the DRAINMOD model. However, in regions where soil analyses are carried out for some essential chemical-physical properties, the poor availability of data on hydraulic properties, such as vertical saturated hydraulic conductivity (K_s), can be a serious constraint in DRAINMOD applications. As a possible solution, pedotransfer functions (PTFs) have been proposed to estimate K_s indirectly from surrogate data (Bouma, 1989; Wösten *et al.*, 2001). Schaap *et al.* (2001) developed the ROSETTA pedotransfer model, which is able to estimate K_s from more easily measured soil properties.

Artificially drained watersheds represent a complex network of ditches that connect individual drained fields with the main stream, where NO_3-N loads from the fields are routed through the stream network to reach the watershed outlet. How to best describe the hydrological and nitrogen processes involved in these areas for planning BMPs to reduce nitrate loading has been the subject of great discussion during recent decades. In modelling nitrate losses from drained agricultural land, it is particularly important to define the appropriate scale to represent these processes. Daren *et al.* (2006) argue that comparative nutrient export information for land management alternatives to prevent excess nitrate loading to water bodies is better provided by estimated values at the watershed scale. However, Birgand *et al.* (2007) noted that the key to nutrient management at the watershed scale is the understanding and quantification of the fate of nutrients, both at the field scale and after they have entered the aquatic environment.

On the other hand, Becker & Braun (1999) indicated that different forms and degrees of heterogeneity need to be considered in hydrological modelling at watershed scale. They applied a disaggregation of the land surface into subareas of uniform behaviour, which can be considered as separate modelling units. For example, the field may be considered as the modelling unit in artificially drained land, where the drainage system connects the outflow and nitrogen losses from individual fields with the stream network in the watershed. This connection between fields and watershed may be made using a framework that integrates field-scale nitrogen models, such as DRAINMOD-N II, with geographical information systems (GIS). Di Luzio *et al.* (2004) noted that such integration of different components (models and GIS) offers a potential synergy that appears to be the key feature for effective understanding and interpretation of these complex hydrological processes associated with water quality assessment at the watershed scale.

Another important point is to define the level of detail required in the model to give a realistic representation of these processes, which should be linked to the available measurements made on the study area. However, when nitrate losses are simulated at watershed scale, the modeller must accept that some processes are not fully understood and cannot be modelled with sufficient accuracy (Quinn, 2004). Beven (2008) noted that optimisation of environmental models cannot be considered a good strategy when the optimum model found may depend on input and model structural errors, and proposed the Generalised Likelihood Uncertainty Estimation (GLUE) methodology for calibration and uncertainty estimation in distributed hydrological models.

In Sweden, determination of nitrate loads from drained agricultural land requires additional knowledge of hydrological and nitrate transport processes and appropriate modelling for land use planning at different scale, which may not be available at present.

2 Objectives

The overall aim of this thesis was to evaluate the effects of temporal and spatial variability in water discharge and nitrogen loads from drained agricultural land at field and watershed scale by modelling the processes involved.

Specific objectives were to:

1. Evaluate the feasibility of running the DRAINMOD hydrological model with ROSETTA-estimated soil hydraulic properties at field scale.
2. Evaluate the DRAINMOD-N II model for predicting outflows and NO_3-N loads at field scale.
3. Develop an integrated framework (Arc Hydro-DRAINMOD) to estimate discharge and NO_3-N loads at watershed scale.
4. Evaluate the Arc Hydro-DRAINMOD for predicting water discharge and NO_3-N loads at watershed scale.
5. Estimate uncertainties of the Arc Hydro-DRAINMOD inputs using the GLUE methodology; and use the GLUE results to carry out a sensitivity analysis of the most important parameters in Arc Hydro-DRAINMOD.

3 Background

Armstrong & Burt (1993) noted that at all scales, the movement of nitrate is intimately associated with the movement of water. Thus when hydrological models are utilised to study nitrate dynamics in agro-ecosystems at different scales, the first stage in the modelling of nitrate loads should be modelling of the water fluxes. To facilitate the applicability of these models, additional components, such as GIS and pedotransfer functions, may be included. It is widely accepted that rivers can reduce downstream nitrate concentrations (Saunders & Kalff, 2001). Therefore, nitrate removal in the stream network should be considered in modelling nitrate loading at watershed scale. The uncertainty that arises in modelling environmental systems is an issue of great current relevance to the impacts of pollutant transport and sustainable resource management, which should be an intrinsic part of any modelling approach (Beven, 2008). Thus in this section brief descriptions of the most important topics relating to water discharge and N modelling are presented, with examples about the components used in this study: Arc Hydro, DRAINMOD, DRAINMOD N-II, GIS and ROSETTA.

3.1 Hydrological and nitrogen modelling

Klemeš (1986) defined a hydrological model as a mathematical model aimed at synthesising a continuous record of some hydrological variable *Y*, for a period *t*, from available current records of other variables *X*, *Z*, *etc*. These models are based on theoretical equations and can integrate reasonable spatial and temporal changes in the natural system. For example, some hydrological models can predict water flows in response to water management systems by evaluating the effects of system design on crop yields and hydrology. There are a number of these hydrological models, for instance DITCH (Armstrong, 2000) and SWATRE (Belmans *et al.*, 1983). Other models have incorporated the effects of water management practices, such as DRAINMOD (Skaggs, 1978, 1999).

DRAINMOD is a field-scale computer simulation model that characterises the response of the soil water regime to various combinations of surface and subsurface water management, such as surface drainage, subsurface drainage, controlled drainage and subirrigation. The model simulates the effects of water management on groundwater level by performing a one-dimensional water balance at the midpoint between adjacent drains. The water balance includes routines to simulate surface and subsurface drainage, infiltration and evapotranspiration. It has been successfully tested under a wide range of soil, crop and climate conditions (Cooper & Fouss, 1988; Mostaghimi *et al.*, 1989; Cox *et al.*, 1994; Singh *et al.*, 2006).

Most of the hydrological models have limited application in seasonally cold regions due to the lack of a freezing and thawing component that considers the effects of these processes on the soil water regime. However, some models have been modified for cold conditions, such as DRAINMOD (Luo *et al.*, 2000) and ADAPT (Alexander, 1988).

The modified DRAINMOD for cold conditions (Luo *et al.*, 2000) uses daily hydrological predictions as in the original model, estimates thermal properties as a function of profile depth and numerically solves the heat flow equation to predict a soil temperature profile. When freezing conditions are indicated by below zero temperatures, the model calculates average ice content in the soil profile and modifies soil hydraulic conductivity and infiltration rate accordingly. Recorded precipitation is separated as rain and snow when daily average air temperature is above or below a rain/snow dividing base temperature. Snow is predicted to accumulate on the ground until air temperature rises above a snowmelt base temperature. Soil surface temperature is recalculated when snow cover exists. Daily snowmelt water is added to rainfall, which may infiltrate or run off, depending on the soil freezing conditions. DRAINMOD has been tested under cold climates in the USA (Jin & Sands, 2003), Canada (Wang *et al.*, 2006a), Turkey (Luo *et al.*, 2001) and Sweden (Wesström, 2002), and predicted values are generally found to agree well with field data.

Several complex models are available to predict the movement and fate of nutrients and pesticides at field scale, for example GLEAMS (Leonard *et al.*, 1987) and CREAMS (Knisel, 1980). However, only a few models can be applied to measure the effects of drainage system design and management on losses of agricultural chemicals in shallow groundwater level soils, such as DRAINMOD-N II (Youssef *et al.*, 2005).

The current DRAINMOD-N II version 6.0 (Youssef *et al.*, 2005) is a field-scale, process-based model that was developed to simulate N dynamics and turnover in the soil-water-plant system under different management practices and soil and environmental conditions. In DRAINMOD-N II, the water balance calculations are computed as in the original DRAINMOD model (Skaggs, 1978, 1999) and include freezing, thawing and snowmelt components (Luo *et al.*, 2000). The DRAINMOD-N II model considers a detailed N cycle that includes atmospheric deposition, application of mineral N fertilisers including urea and anhydrous ammonia (NH_3), soil amendment with organic N (ON) sources including plant residues and animal waste, atmospheric N_2 fixation by leguminous crops, plant uptake, organic C (OC) decomposition and associated N mineralisation/immobilisation, nitrification, denitrification, volatilisation of NH_3 and N losses via subsurface drainage and surface runoff. Youssef (2003) developed the DRAINMOD-N II model using data from an artificially drained agricultural site located in North Carolina, USA. Results of this study showed the potential of DRAINMOD-N II to predict N losses from drained agricultural land at field scale. Moreover, DRAINMOD-N II has been successfully calibrated and validated for predictions of N concentrations in drainage water in Germany (Bechtold *et al.*, 2007) and Illinois, USA (David *et al.*, 2009).

At watershed scale, the different hydrological models have different degrees of complexity that range from simplified lumped parameters to a more physically-based distributed approach (Borah & Bera, 2003). Lumped models treat the whole of an area as a single accounting unit, while distributed models treat the area as a spatially variable physical system with various functioning hydrological units. Compared with lumped models, Bathurst & O'Connell (1992) highlighted the advantages of distributed models, which considered the spatial variability, for studying the effects of land use on watershed nutrient losses.

In Sweden, computer models used to predict the movement and fate of nutrients from agricultural land to water bodies at different scales include HBV-N (Arheimer & Brandt, 2000; Andersson & Arheimer, 2003), SOILN (Johnsson *et al.*, 1987; Hoffmann *et al.*, 2000; Blombäck *et al.*, 2003) and SOILNDB (Johnsson *et al.*, 2002; Kyllmar *et al.*, 2005). However, these models do not consider the effect of water management practices, drainage and irrigation on hydrology and nutrient losses.

3.2 Modelling and GIS

The widespread availability of digital geographical data opens up new opportunities for using models in watershed planning (Frankenberger *et al.*, 1999). The applicability of field-scale models can be extended to a watershed scale by combining them with a Geographical Information System (GIS) (Sui & Maggio, 1999; McKinney & Cai, 2002), where GIS is transformed from a simple query and visualisation tool to a powerful analytical and spatially distributed modelling tool. Thus the integration of GIS and simulation models within a common and interactive graphical user interface produces more powerful, easy-to-use and comprehensible planning and analysis of information systems (Sweeney, 1999).

The geographical analysis abilities of GIS can be used to calculate indicators that represent the status and trends in the physical, biological and chemical properties of water in the watershed (Aspinall & Pearson, 2000). For instance, studies in the USA have reported that a combination of the field-scale DRAINMOD model and GIS had acceptable accuracy for estimating water flow and NO_3-N concentrations at watershed scale, based on field-scale predictions (Northcott *et al.*, 2002; Sammons *et al.*, 2005; Fernandez *et al.*, 2006). Northcott *et al.* (2002) and Sammons *et al.* (2005) coupled DRAINMOD with GIS to simulate the hydrological response of a tile-drained watershed. Northcott *et al.* (2002) subdivided a tile-drained watershed into uniform cells of 16 ha and ran DRAINMOD on each cell with inputs based on the individual characteristics of each cell. The result was a distributed parameter model based on the water balance of DRAINMOD that accounted for surface runoff, subsurface tile flow and stream baseflow. In another study, Fernandez *et al.* (2006) developed a tool that integrated DRAINMOD, a generalised spatially distributed network model and GIS. This tool was developed using the network model as a basis for drainage network routing. The tool considered spatially distributed parameters and outflows from contributing areas, which were routed directly through the drainage network to the outlet.

Maidment (2002) developed the Arc Hydro data model, which operates in the ArcGIS environment for representing surface water systems. A detailed description of Arc Hydro can be found in Maidment (2002) and ESRI (2007). It provides a basic database design and sets of tools to help in the creation, manipulation and display of Arc Hydro features and objects within the ArcGIS environment, such as river network, drainage areas and related temporal information. Moreover, Arc Hydro allows hydrological models to be linked with GIS through a common data storage system. For instance, Whiteaker *et al.* (2006) present two cases of how hydrological models connected with a schematic network generated by Arc Hydro tools can be used for simulating rainfall-runoff and bacterial loading from watersheds. Recently, Fürst & Hörhan (2009) used the Arc Hydro data model to represent the stream hierarchy of watersheds in Austria.

3.3 Pedotransfer functions

Direct measurements of hydraulic properties are time-consuming and therefore costly. As an alternative, pedotransfer functions (PTFs) have been proposed to indirectly estimate soil hydraulic properties from more easily measured and more readily available soil properties, such as particle-size distribution, organic matter content and bulk density (Cornelis *et al.*, 2001; Givi *et al.*, 2004; Mermoud & Xu, 2006).

Common PTFs include regression models developed from existing soil databases (*e.g.* Tietje & Tapkenhinrichs, 1993; Vereecken, 1995). However, practical application of most PTFs is hampered by their very specific data requirements and they usually provide estimations with a modest level of accuracy (Schaap *et al.*, 2001).

Artificial neural network (ANN) analyses are becoming a common tool to establish empirical PTFs (Pachepsky *et al.*, 1996; Schaap & Leij, 1998; Minasny *et al.*, 1999). An ANN consists of a box containing single computational elements called neurons, which exist in layers and are dynamically interconnected by synapses (Gupta & Yan, 2006). The advantages of ANN, compared with traditional PTFs, are that ANN requires no *a priori* model concept and that it has the ability to mimic the behaviour of complex systems by varying the strength of influence of network components on each other as well as its range of choices of structures of interconnections among components (Schaap *et al.*, 2001; Wösten *et al.*, 2001).

To facilitate application of ANN, Schaap *et al.* (2001) developed the ROSETTA model, which is capable of estimating soil hydraulic properties indirectly from surrogate data available in soil surveys, such as texture class, soil texture, bulk density and one or two water retention points. ROSETTA is capable of predicting van Genuchten (1980) water retention parameters and saturated hydraulic conductivity (K_s), as well as unsaturated hydraulic conductivity parameters based on the Mualem (1976) pore-size model. Schaap *et al.* (2001) obtained K_s values and corresponding predictive soil properties from databases of North America and Europe, which included 1306 soil samples.

PTFs in combination with soil databases offer a quick and easy way to derive the soil hydraulic parameters that are necessary to run hydrological models at different scales. For example, ROSETTA is included as a sub-model in DRAINMOD for estimating residual and saturated volumetric water contents (θ_r and θ_s, respectively), K_s and other parameters, which are required in the DRAINMOD routine for creating a soil file. Singh *et al.* (2006) ran DRAINMOD with hydraulic property inputs produced using ROSETTA for clay loam conventional drainage plots in Iowa, and found good agreement when comparing DRAINMOD-simulated and observed overall drainage outflows. At watershed scale, Christiaens & Feyen (2001) used PTFs in a watershed distributed modelling approach, which proved to be a valid method of estimating soil hydraulic properties.

3.4 Nitrogen removal from stream networks

The sum of N inputs to the stream network in a watershed usually exceeds loads discharged at the outlet, with the stream network acting as a filter retaining or removing N by processes such as denitrification, sedimentation, and plant and microbial uptake (assimilation) (Billen *et al.*, 1991). A number of studies have calculated that a substantial amount of N can be removed from the network of rivers draining watersheds, with values ranging from 10% to 76% of the N input to the rivers (Saunders & Kalff, 2001; Seitzinger *et al.*, 2002; Lepistö *et al.*, 2006; Birgand *et al.*, 2007; Appelboom *et al.*, 2008).

Some researchers have reported denitrification to be the dominant nitrate (NO_3^-) loss process in rivers, where NO_3^- is permanently removed through the formation and release of N_2 (g) and N_2O (g) into the atmosphere (Saunders & Kalff, 2001; Seitzinger, 1988).

The N removal rate in the stream network has been included in several modelling approaches at watershed scale. It has been represented either as a percentage of the total N inputs (Bhuyan *et al.*, 2003; León *et al.*, 2004) or as an exponential decay model (Skop & Sørensen, 1998; Fernandez *et al.,* 2002, 2006). However, these approaches did not include temperature as a factor that affects the N removal rate, although temperature has been identified as a key factor in N denitrification experiments (Dawson & Murphy, 1972; Appelboom *et al.*, 2006). The Arrhenius equation may be used to represent the positive relationship between denitrification rate and temperature (Dawson & Murphy, 1972).

3.5 Uncertainty and sensitity analysis in hydrological modelling

Although most hydrologic models are largely physically based, they are not capable of describing the exact hydrological and chemical processes that occur under natural conditions (Haan *et al.*, 1995). Furthermore, several authors have noted that uncertainty analysis (UA) and sensitivity analysis (SA) are essential prerequisites for model building, providing information on the pedigree of model predictions to users and decision-makers (Crosetto *et al.*, 2000; Saltelli *et al.*, 2000; Beven, 2008). While UA aims to measure the overall uncertainty associated with the model response as a result of uncertainties in the model input, SA studies how the variations in the model output can be apportioned to different sources of variation. Several methods of UA and SA are available, such as those presented in comprehensive reviews by Hamby (1994), Saltelli *et al.* (2000) and Manache & Melching (2008).

3.5.1 Uncertainty analysis

One of the most common methods of UA is Monte Carlo simulation (MC), which is based on performing multiple evaluations of the model with randomly selected model inputs (Crosetto *et al.*, 2000). It is particularly useful when the outputs of the model depend non-linearly on the inputs and parameter values, as is the case in most environmental models, so that propagation of uncertainties is not possible (Beven, 2008). However, in a high-dimensional model space it may be difficult to make sufficient samples to represent the shape of the response surface, as is required in MC, due to computational limitations.

Another UA method is first order analysis (FOA), which produces estimates of the mean and variance of a model response (Haan *et al.*, 1995). It is simple to apply and computationally inexpensive, but the disadvantage is that even for mildly non-linear models the results may be rather inaccurate (Beven, 2008). Haan & Skaggs (2003) conducted UA on DRAINMOD using data from a drainage experiment field in North Carolina, USA. They used MC and FOA methods to determine the uncertainty in model inputs, and found that lateral saturated hydraulic conductivity (LK_s) accounted for 81% and 62% of the uncertainty in predicted annual subsurface drainage volume in conventional and controlled drainage systems, respectively.

At watershed scale, Fernandez *et al.* (2006) evaluated the impact of uncertainty in DRAINMOD-GIS inputs on predicted discharge and nitrate loads using MC and FOA methods. They found that uncertainty in stream velocity, decay coefficient and field exports significantly contributed to the uncertainty in predicted model outputs.

Other authors have used Bayesian analysis to estimate uncertainty in hydrological modelling (Engeland *et al.*, 2005; Kuczera *et al.*, 2006; Yang *et al.*, 2007). The Bayesian method estimates a probability density for the model parameters conditioned on observations, where the uncertainty is calculated around the optimal value of one objective function (Engeland & Gottschalk, 2002). However, Beven (2008) noted that a disadvantage of Bayesian analysis is the assumption of a formal model of the errors, which is usually difficult to verify if all sources of errors are lumped.

In contrast, Beven & Binley (1992) proposed a new method for UA in distributed models, the Generalised Likelihood Uncertainty Estimation (GLUE) methodology. The method involves handling the modelling errors and does not force assumptions about the error structure. The starting point for the GLUE concept is rejection of the idea of an optimum parameter set in favour of the concept of equifinality (Beven & Freer, 2001). Beven (2001) noted that the equifinality concept recognises that under the limited measurements available in any application of a distributed hydrological model, it should be accepted that there are many different model structures and parameter sets that can be used in simulating the available data. Beven & Freer (2001) noted that any effects of model non-linearity, covariation of parameter values and errors in model structure input data or observed variables with which the simulations are compared are considered within this procedure. The general requirements of the GLUE procedure may be summarised as follows: i) a formal definition of a likelihood measure; ii) an appropriate definition of the prior parameter distribution; iii) a procedure for using likelihood weights in uncertainty estimation; iv) a procedure for updating likelihood weights recursively as new data become available and v) a procedure for evaluating uncertainty such that the value of additional data can be assessed.

The GLUE methodology has recently been used to calibrate and perform UA on a variety of hydrological distributed models at watershed scale, such as HBV-NP (Lindström *et al.*, 2005), LISFLOOD-WB (Mo *et al.*, 2006), MIKE-SHE (Blasone *et al.*, 2008), MOUSE (Thorndahl *et al.*, 2008), SWAT (Arabi *et al.*, 2007), and TOPMODEL (Beven & Freer, 2001; Choi & Beven, 2007).

Moreover, in a field drainage experiment in Indiana, USA, Wang *et al.* (2006b) performed UA using the GLUE procedure to identify the main sources of uncertainty in DRAINMOD predictions. Their GLUE results showed that the observed annual drain outflows fell well within the confidence intervals (5 and 95%), although some of the daily and monthly observations did not.

3.5.2 Sensitivity analysis

The simplest method of SA is the one-factor-at-a-time (OAT) approach, which consists of repeatedly varying one parameter at a time while assuming that all other parameters are fixed (Saltelli *et al.*, 2005). van Griensven *et al.* (2006) proposed a modification to the current OAT method by including Latin hypercube sampling (LH). The concept of LH is based on MC simulations but uses a stratified sampling approach that allows efficient estimations of the output statistics. For instance, Wang *et al.* (2005) performed SA using the LH-OAT method in DRAINMOD-N II using data from an experimental field in North Carolina, USA. They found that DRAINMOD-N II was most sensitive to denitrification parameters, especially those controlling temperature effects on process rate. Their study also indicated that DRAINMOD-N II is mildly sensitive to the parameters controlling organic carbon decomposition and associated N mineralisation/immobilisation.

Another simple method of SA is to use a sensitivity index, such as absolute or relative coefficients that can be used to examine the relative sensitivity of different factors in the model space (Haan *et al.*, 2005). In this approach, a sensitivity index calculates the output percentage difference when varying one input parameter from its minimum value to its maximum value (Hamby, 1994). Although sensitivity measures might be a good preliminary guide to the sensitivity of individual inputs, they have problems in exploring the way in which sensitivity might vary through the model space (Beven, 2008). In the aforementioned study by Haan & Skaggs (2003), SA included in DRAINMOD using sensitivity indexes showed that LK_s, maximum surface storage and residual and saturated volumetric water content were the most sensitive parameters.

Saltelli *et al.* (1999) proposed the extended Fourier amplitude sensitivity test (extended FAST), which allows the total contribution of each input factor to output variance to be accounted for. In the study by Wang *et al.* (2006b), use of the extended FAST method showed that DRAINMOD results were most sensitive to K_s of the restrictive soil layer and LK_s of the deepest soil layer.

It is also possible to use the GLUE results to perform an SA. This methodology was proposed by Hornberger & Spear (1981) and adapted by Beven & Binley (1992) to consider the likelihood weights for the behavioural simulations. This SA performs a comparison between cumulative distributions of behavioural and non-behavioural simulations, where the SA results can be evaluated using sensitivity plots of the cumulative distributions or a measure of sensitivity, such as the Kolmogorov-Smirnov d-statistic (d_{K-S}) (Beven, 2008).

4 Materials and Methods

This section briefly describes datasets and methods used to simulate water discharge and nitrate loads at field and watershed scale at two sites in south-east Sweden. The statistical, uncertainty and sensitivity analysis methodologies used to evaluate model performance are also described.

4.1 Site description and measures

Field-scale simulations (Papers I and II) used data from a drainage experiment site established at Gärds Köpinge (south-east Sweden, 55°56´N, 14°10´E, in the county of Skåne). One plot with conventional subsurface drainage (CD/Plot 3) and two plots with controlled drainage (CWT1/Plot 2 and CWT2/Plot 4) were used in the simulations. The plot size was 0.14 ha.

Watershed-scale simulations (Papers III and IV) used data from the Kleva river watershed located at Mörbylånga on the island of Öland (south-east Sweden, 55°31´N, 16°23´E, in the county of Kalmar). It is a 734 ha, artificially drained watershed consisting of 95 agricultural fields ranging in area from 0.2 to 32 ha. The watershed is characterised by flat topography, with average slope less than 1%. Steep slopes >10% only occur in the hills located on the eastern watershed boundary where the maximum ground elevation of 50 m a.s.l. is found. The watershed is drained by the Kleva river, which is divided into two branches, and a network of field ditches. The location of the Gärds Köpinge experimental site and the Kleva river watershed in south-east Sweden and layouts are shown in Figure 1.

4.1.1 Soil and nitrogen measurements

The soil at Gärds Köpinge is characterised by distinct textural horizons: a loamy sand topsoil (0-40 cm), weakly structured with an organic matter content of 5%, overlies a sand layer (40-100 cm) with low organic matter content (Wesström, 2006). Below 1 m depth there is a clay layer, which effectively restricts downward seepage.

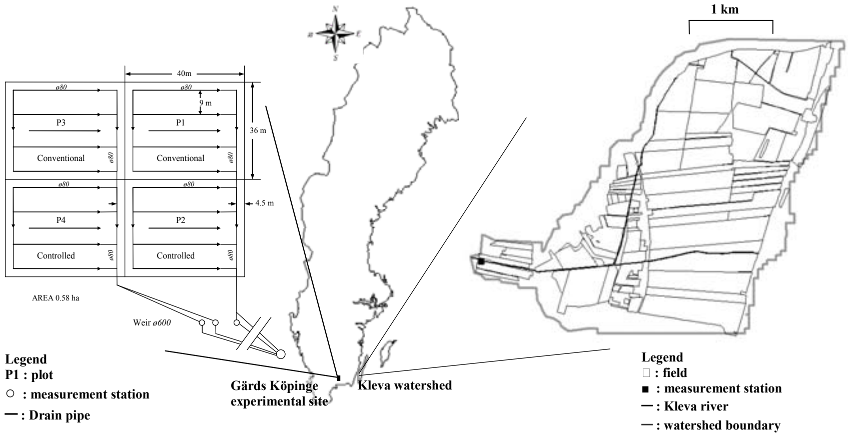

Figure 1. Location of the Gärds Köpinge experimental site and Kleva river watershed on Öland island, off the south-east coast of Sweden, and layouts.

At Gärds Köpinge, soil bulk density (ρb), vertical saturated hydraulic conductivity (K_s) and soil water retention were determined using standard laboratory procedures on undisturbed soil cores in steel cylinders (7.2 cm in diameter, 10 cm in height) taken at 10 cm intervals down to 100 cm depth (Andersson, 1955). Soil water retention was measured at the pressure heads -0.5, -1.5, -3, -5, -10, -33, -60 and -1500 kPa. K_s was measured 1 h and 24 h after saturated water flow at a constant head gradient. In addition, soil texture was determined for 10-cm layers down to 100 cm using the method of sieving and pipetting (Ljung, 1987). Mineral N concentrations (NO_3-N and NH_4-N) in the soil profile were measured three times during the year using a method described by Lindén (1981) at three soil depths: 0-30, 30-60 and 60-90 cm. The samples were stored frozen (-20 °C). After thawing and extraction with 2 M KCl, NO_3-N and NH_4-N were determined using automatic colorimetric methods. Crop biomass was sampled twice during the growing season in each plot, for determination of yield and N content.

The Kleva river watershed consists mainly of coarse-textured soils developed from glacial drifts, with a smaller area of organic soils derived from peat next to the outlet. The watershed is underlain by sedimentary rocks such as limestone, alum shale, sandstone and clay shale.

4.1.2 Climate

Gärds Köpinge and the Kleva river watershed have a Marine West Coast climate (Cfb) according to the Köppen-Geiger system (Peel *et al.*, 2007).

Gärds Köpinge has a mean annual air temperature of 7.6 °C and mean annual precipitation of 562 mm (using 1961-1990 data from a meteorological station at Kristianstad).

The Kleva river watershed has a mean annual air temperature of 7.4 °C and mean annual precipitation of 475 mm (using 1961-1990 data from a meteorological station at Mörbylånga on Öland).

At both sites, potential evapotranspiration (PET) was calculated using the FAO Penman-Monteith combination equation (Allen *et al.*, 1998). Data on snow events were obtained from meteorological network stations next to Gärds Köpinge and Kleva river watershed.

4.1.3 Crops

At Gärds Köpinge, all plots are part of a conventional Swedish farming system, which includes winter wheat (*Triticum aestivum L.*) and sugarbeet (*Beta vulgaris L.* ssp. *vulgaris*) followed by two years of spring barley (*Hordeum vulgare L.*) in the 4-year crop rotation.

In the Kleva river watershed, crop data for the different fields were obtained from the Swedish Board of Agriculture. The main crops cultivated in the watershed are winter wheat, spring barley, sugarbeet, peas (*Pisum sativum L.*), potatoes (*Solanum tuberosum L.*) and beans (*Phaseolus vulgaris L.*). Perennial ryegrass (*Lolium perenne L.*) is used for cultivated grassland.

At both sites, crops are grown with conventional tillage, fertiliser and pest management practices typical of the region.

4.1.4 Water discharge and nitrogen measurements

At Gärds Köpinge, the drain outflow rate from each plot was measured continuously. In the Kleva river watershed, discharge measurements were taken continuously by a stream-flow station located at the watershed outlet.

At both sites, samples of drainage water were collected for analysis twice a month during flow periods. The water was analysed for NO_3-N according to Swedish standards. Daily values of NO_3-N concentrations were obtained by linear interpolation of the measured values. Fluxes of NO_3-N by discharge were calculated by multiplying daily discharge values by daily concentration values.

4.1.5 Time scale

In all simulations, a monthly time scale was used as the unit to represent temporal characteristics of hydrological and nitrogen data. In Papers II, III and IV, a 'Period' time scale was used, which corresponded to different hydrological years when complete datasets were available to run the models. Although in Papers III and IV daily simulations were performed, these were aggregated to a monthly time scale to facilitate statistical analysis and comparison. Only in Paper III was the model performance evaluated on a daily basis during high discharge events. The times scales used in Papers I-IV are presented in Table 1.

Table 1. *Times scales used in Papers I-IV*

Paper	Year	N^a	Period[b]					
			1	2	3	4	5	6
I	2001-2004	23-29	-	-	-	-	-	-
II	2002-2004	36	Jan 02-Jun 02	Jul 02-Jun 03	Jul 03-Jun 04	Jul 04-Dec 04	-	-
III	2003-2008	45	Oct 03-Jun 04	Jul 04-Jun 05	Jul 05-Sep 05	Jan 06-Jun 06	Jan 07-Jun 07	Jul 07-Mar 08
IV	2003-2007	42	Oct 03-Jun 04	Jul 04-Jun 05	Jul 05-Sep 05	Jan 06-Jun 06	Jan 07-Jun 07	Jul 07-Dec 07

[a] N = number of months

[b] Periods correspond to different hydrological years

4.2 Modelling outflow and nitrogen loads at field scale

4.2.1 Estimation of hydraulic soil properties by ROSETTA (Paper I)

Measured soil parameters at three soil depths (0-40 cm, 40-100 cm and 100-130 cm) were used as inputs in ROSETTA to estimate K_s. These parameters were assembled into four input datasets for ROSETTA through a hierarchical approach from limited information (USDA textural class) to more extended sets of soil information that included texture, bulk density (ρb), and water retention at -33 kPa (θ_{33kPa}) and -1500 kPa ($\theta_{1500kPa}$) (Table 2).

These five datasets (H0 to H4) were used to develop drained volume-groundwater level-upward flux relationships and Green-Ampt parameters using the SOILPREP programme in DRAINMOD.

Table 2. *Combinations of soil parameter data used as input in DRAINMOD*

Dataset	Description of data
H0	Laboratory-measured K_s
H1	ROSETTA-estimated K_s from texture class
H2	ROSETTA-estimated K_s from soil texture
H3	ROSETTA-estimated K_s from soil texture and ρb
H4	ROSETTA-estimated K_s from soil texture, ρb, θ_{33kPa} and $\theta_{1500kPa}$

4.2.2 DRAINMOD inputs (Papers I,II)

DRAINMOD inputs included climate data, soil properties, crop parameters and drainage parameters, which were obtained from measured data at the Gärds Köpinge field experiment. Additional input data were required to predict soil freezing, thawing and snow accumulation in DRAINMOD for cold conditions, and these were estimated from measured data at the experimental site according to Luo *et al.* (2000). Table 4 in Paper I lists some selected input data required from drainage system design, crop production and soil temperature, while Table 2 in Paper II shows soil property inputs.

4.2.3 DRAINMOD-N II inputs (Paper II)

Soil inputs were obtained from soil samples taken from the experimental site. Crop production and biochemical composition of barley, sugarbeet and wheat were set to field-measured crop data at Gärds Köpinge or obtained from ranges published in the literature (see Tables A1-A4 in appendix). DRAINMOD-N II inputs for N transport and transformation processes are presented in Table 3, and inputs for organic matter parameters in Table 4.

Table 3. *Transport and transformation parameters used in DRAINMOD-N II*

Transport and transformation parameter		
Longitude dispersivity (cm)		5
Tortuosity		0.5
Critical pH		7.5
	Nitrification	Denitrification
V_{max} (µg N g^{-1} soil d^{-1})	9	4
K_m	170	30
Optimum temperature (ºC)	20	25
Threshold water-filled pore space	–	0.8
Optimum water-filled pore space range	0.5 to 0.6	–

Table 4. *Organic matter parameters used in DRAINMOD-N II*

Organic matter parameter	Value		
Optimum temperature (C)		30	
Optimum WFPS range		0.5 to 0.6	
Litter pools	C/N ratio	Decomposition rate (d^{-1})	
Surface structural	150	1.0685×10^{-2}	
Surface metabolic	15	4.0548×10^{-2}	
Surface microbes	8	1.6438×10^{-2}	
Below-ground structural	150	1.3425×10^{-2}	
Below-ground metabolic	15	5.0685×10^{-2}	
SOM pools	Initial OC assigned to pool (%)	C/N ratio	Decomposition rate
Active	2	15	2.0000×10^{-2}
Slow	28	20	5.4795×10^{-4}
Passive	70	10	1.2329×10^{-5}

4.2.4 Model calibration and validation (Papers I,II)

Data from plot with conventional drainage (CD) was used for the calibration process, while datasets from the other two plots with controlled drainage (CWT1 and CWT2) were used for model validation. The models were calibrated sequentially for the hydrological and N components.

To evaluate the feasibility of running DRAINMOD with K_s input produced using ROSETTA, laboratory-measured K_s values were considered for adjusting the subsurface drainage flow. Drainage outflow data measured during 29 months were used in CD, while 23 months were considered in CWT1 and CWT2. Once the hydrological calibration and validation processes had been completed, a set of DRAINMOD simulations was conducted using ROSETTA-estimated K_s values (H1, H2, H3 and H4), which used the same parameters characterising the crop, drainage system parameters and climate data.

The lateral saturated hydraulic conductivity (LK_s) values used in DRAINMOD simulations were obtained through model calibration, which assumed LK_s values to be in the range of 1 to 4 times K_s values. A pareto preference ordering procedure (Yapo *et al.*, 1998; Khu & Madsen, 2005) was applied to identify pareto-optimal solutions for LK_s values using the modelling efficiency (E) as performance measure during calibration. The pareto-optimal set approach is a set of models with different parameters sets that are illustrated along a line called the pareto front, which reflects the trade-off between E values (Beven, 2008).

In DRAINMOD-N II, calibrated N parameters were manually adjusted by visually and statistically comparing observed and simulated drainage outflows and NO_3-N losses in subsurface drains according to Youssef *et al.* (2006). This included transport, nitrification and denitrification as calibrated input parameters.

4.2.5 Statistical analysis (Papers I,II)

In model calibration/validation, monthly observed and simulated drainage outflows and NO_3-N losses in subsurface drains were compared by calculating some of the following likelihood measures:

Mean absolute error

The mean absolute error (*MAE*) describes the difference between the model simulations and observations in the units of the variable (Legates & McCabe, 1999), according to:

$$MAE = \frac{1}{n}\sum_{i=1}^{n}\left|O_i - S_i\right| \qquad \text{(Eq. 1)}$$

where O_i is the individual observed value at time *i*, S_i is the individual simulated value at time *i* and *n* is the number of paired observer-simulated values. The value of *MAE* should be equal to zero for a model showing a perfect fit between the observed and predicted data.

Modelling efficiency

The modelling efficiency or coefficient of efficiency (*E*) represents the ratio between the mean square error (*MSE*) and the variance in observed data (s^2), multiplied by the number of paired observer-simulated values (*n*) and then subtracted from unity (Nash & Sutcliffe, 1970), given by:

$$E = 1.0 - n\frac{MSE}{s^2} = 1.0 - \frac{\sum_{i=1}^{n}\left(O_i - S_i\right)^2}{\sum_{i=1}^{n}\left(O_i - O'\right)^2} \qquad \text{(Eq. 2)}$$

where O_i is the individual observed value at time *i*, S_i is the individual simulated value at time *i* and *O'* is the mean observed value. The value of *E* ranges from minus infinity to 1.0, where an *E* of 1.0 represents a perfect prediction and lower values indicate less accurate agreement between the model and observations. Thus a value of zero for *E* indicates that *O'* is as good a predictor as the model, whereas negative values indicate that the observed mean is a better predictor than the model. In this study the general performance rating for E values in monthly comparisons proposed by Moriasi *et al.* (2007) was used, as in shown in Table 5.

Table 5. *Modelling efficiency (E) performance rating for monthly comparisons (Moriasi et al., 2007)*

Performance rating	E
Very good	$0.75< E \leq 1.00$
Good	$0.65< E \leq 0.75$
Satisfactory	$0.50< E \leq 0.65$
Unsatisfactory	$E \leq 0.50$

Legates & McCabe (1999) noted that E is overly sensitive to extreme values and proposed the modified modelling efficiency (E'). They adjusted E to reduce the effect of square terms by using absolute values as:

$$E' = 1.0 - \frac{\sum_{i=1}^{n} |O_i - S_i|}{\sum_{i=1}^{n} |O_i - O'|} \qquad \text{(Eq. 3)}$$

Index of agreement

The index of agreement (d) represents the ratio between the mean square error (MSE) and the potential error (PE), multiplied by the number of paired observer-simulated values (n) and then subtracted from unity (Willmott *et al.*, 1985) according to:

$$d = 1.0 - n\frac{MSE}{PE} = 1.0 - \frac{\sum_{i=1}^{n} (O_i - S_i)^2}{\sum_{i=1}^{n} (|S_i - O'| + |O_i - O'|)^2} \qquad \text{(Eq. 4)}$$

where O_i is the individual observed value at time i, S_i is the individual simulated value at time I and O' is the mean observed value. The value of d varies from 0.0 to 1.0, with higher values indicating better agreement with the field observations (Willmott *et al.*, 1985). Legates & McCabe (1999) noted that the interpretation of d closely follows the interpretation of the determination coefficient (R^2) for most values encountered.

Legates & McCabe (1999) also argued that d is sensitive to outliers and, similarly to E, proposed a modified index of agreement (d') as:

$$d' = 1.0 - \frac{\sum_{i=1}^{n} |O_i - S_i|}{\sum_{i=1}^{n} (|S_i - O'| + |O_i - O'|)} \qquad \text{(Eq. 5)}$$

Percent-normalised error

The percent-normalised error (*NE*) represents the percent error of the simulated values (Janssen & Heuberger, 1995) as:

$$NE = 100\frac{\sum_{i=1}^{n} S_i - \sum_{i=1}^{n} O_i}{\sum_{i=1}^{n} O_i} \quad \text{(Eq. 6)}$$

where O_i is the individual observed value at time *i*, S_i is the individual simulated value at time *i* and *n* is the number of paired observer-simulated values.

4.3 Modelling outflow and nitrogen loads at watershed scale

The framework development for simulations of hydrology and nitrogen processes at watershed scale involved integration of the previous evaluations of its components (DRAINMOD, DRAINMOD-N II and ROSETTA) at the Gärds Köpinge field experiment, which had similar climate, soil, crop and management conditions as in the Kleva river watershed.

4.3.1 Arc Hydro-DRAINMOD development (Papers III,IV)

Arc Hydro-DRAINMOD is an integrated framework in which distributed predictions of watershed response are made based on the field-scale hydrological DRAINMOD/DRAINMOD-N II models and the Arc Hydro data model. The GIS software ArcGIS Info 9.2 (ESRI, 2006) is used as a common platform to embed all components and to store data needed as input in the other components. The Arc Hydro data model (Maidment, 2002) describes the drainage patterns in the watershed and connects the DRAINMOD/DRAINMOD-N II outputs from fields to the stream network. The ROSETTA pedotransfer function model (Schaap *et al.*, 2001) is used to estimate soil hydraulic properties required for running the DRAINMOD model. The stream network and watershed boundary are based on DEM file and ArcGIS shapefile (soil texture map, river, ditches and field layout) input data.

Simulations of discharge and NO_3-N load on each field are stored in time series. The time series are then routed from each field to the watershed outlet using a schematic network created by Arc Hydro tools, where the time series from each field are summed through the stream network to predict discharge and NO_3-N load at the watershed outlet.

DRAINMOD and DRAINMOD-N II are also used to simulate the stream baseflow discharge and stream baseflow NO_3-N load, respectively, as a single run that is summed to the stream network at the watershed outlet. Thus the watershed discharge and NO_3-N load that reach the watershed outlet ($load_{received}$) are a combination of DRAINMOD/ DRAINMOD-N II outputs from field simulations and DRAINMOD/ DRAINMOD-N II outputs from stream baseflow simulations.

Finally, the N removal processes (denitrification) that occur in the stream network are considered by using the Arrhenius equation according to Dawson & Murphy (1972) as:

$$k_{den} = k_{c1} \exp(k_{c2} T t) \qquad \text{(Eq. 7)}$$

where k_{c1} is the decay coefficient 1, k_{c2} is the decay coefficient 2 (°C^{-1} day^{-1}), T is the daily average air temperature (°C), and t is the travel time (day). Thus the load that passes through the watershed outlet is reduced according to Eq. (7) as:

$$\mathrm{load}_{passed}(t) = \mathrm{load}_{received}(t)\ k_{den} \qquad \text{(Eq. 8)}$$

where $load_{passed}$ is the downstream NO_3-N load (kg day^{-1}), $load_{received}$ is the upstream NO_3-N load (kg day^{-1}), k_{den} is the denitrification rate constant (Eq. 7), and t is the travel time (day). The framework components and connections are shown in Figure 2.

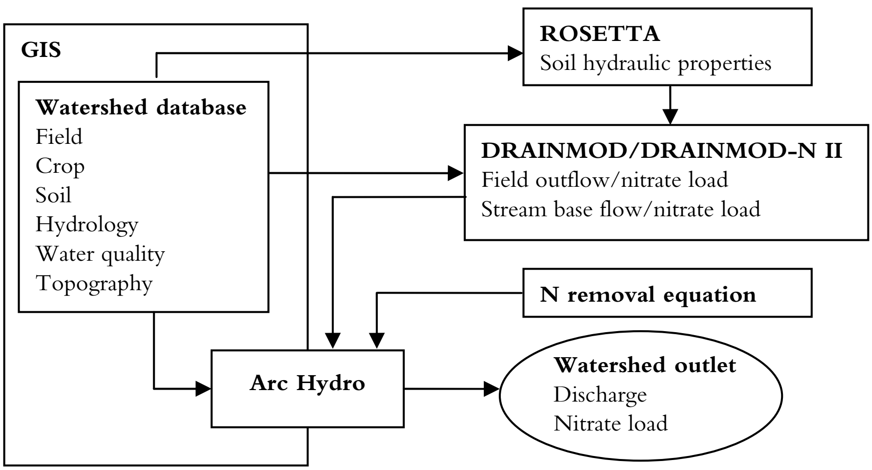

Figure 2. Basic outline of the Arc Hydro-DRAINMOD framework.

4.3.2 Arc Hydro-DRAINMOD inputs for hydrological processes (Paper III)

The DRAINMOD inputs used in this simulation were based on those used in Paper I. Soil hydraulic properties were estimated with the ROSETTA model, which uses USDA textural class as input (see Table 3 in Paper III).

Climatic data were obtained from the Kalmar meteorological station. Information on crop rotation in each field during the study period was obtained from the Swedish Board of Agriculture statistical database (see Table 1 in Paper III).

Crop input data for winter wheat, spring barley, sugarbeet and potatoes were obtained from Paper I and a previous DRAINMOD evaluation in southern Sweden (Wesström, 2002), while data for ryegrass, peas and beans were taken from ranges published in the literature (see Tables A1-A4 in appendix). Crop rotation and management on each field were obtained from data reported by farmers to the Swedish Board of Agriculture in Kalmar county (Jordbruksverket, 2003, 2004a, 2004b, 2005, 2006, 2007).

Drainage system parameters were obtained from field and topographical surveys carried out in the Kleva river watershed (see Table 5 in Paper III). Soil temperature and snow cover predictions required for DRAINMOD were calculated according to methodologies proposed by Luo *et al.* (2000). Some soil temperature and snow accumulation/snowmelt parameters were based on Paper I.

4.3.3 Arc Hydro-DRAINMOD inputs for N processes (Paper IV)

The DRAINMOD-N II inputs used in this simulation were based on those used in Paper II (Tables 3 and 4), and on ranges published in the literature. Soil inputs were obtained from reports on the study area by the Division of Agricultural Hydrotechnics, SLU (see Table 3 in Paper IV). Crop and management parameters used in DRAINMOD-N II simulations were similar to those used in Paper II for winter wheat, sugarbeet and spring barley. For peas, potatoes and ryegrass, crop and management parameter values were obtained from ranges published in the literature (see Tables A1-A4 in appendix). Data on mineral N fertilisation and manure application in each field were obtained from data reported by farmers to the Swedish Board of Agriculture (Jordbruksverket, 2008).

The measured mean daily air temperature and the two decay coefficients were used for nitrate removal estimation (Eq. 7).

4.3.4 Calibration, validation and uncertainty estimation

Arc Hydro-DRAINMOD was run for six periods (Table 1). The first three periods were used for the calibration process, while the last three periods were retained for model validation.

The simulations were carried out in two stages. In the first stage the DRAINMOD model was used in Arc Hydro-DRAINMOD to simulate the watershed discharge (Paper III). In the second stage the nitrogen model DRAINMOD-N II and temperature-dependent NO_3-N removal equations were used in the Arc Hydro-DRAINMOD framework to predict NO_3-N loading (Paper IV).

Arc Hydro-DRAINMOD was calibrated and validated and uncertainty in monthly discharge and NO_3-N load predictions was estimated at watershed scale using the GLUE procedure in the following steps:

Definition of a likelihood measure

The modelling efficiency (E) (Eq. 2) was selected as likelihood function. The likelihood threshold for a model to be considered behavioural can be set to bracket a chosen proportion of the observations (Beven, 2008). In this study, the following likelihood thresholds of acceptability were tested: $E \geq 0.3$, $E \geq 0.4$, $E \geq 0.5$ and $E \geq 0.6$, to determine the threshold ensured to bracket at least 60% of the observations. Thus all the simulations with an E value equal to or greater than the chosen threshold were retained for making predictions in discharge and NO_3-N load and were classified as behavioural simulations. In contrast, all the simulations with an E value lower than the chosen threshold were classified as non-behavioural simulations and given a likelihood of zero.

Definition of the prior parameter distribution

In this study three parameters were calibrated using the GLUE methodology: lateral saturated hydraulic conductivity (LK_s) (six replicates according to the textural classes found in the Kleva river watershed), the distance between the river and the watershed boundary (drain spacing, DS) in the stream base-flow DRAINMOD-simulation, and the decay coefficients (K_{c1} and K_{c2}) in the N removal equation (Eq. 7). The distribution of parameter values to be considered was defined on the basis of some prior knowledge about the system for LK_s and DS, which considered the following two assumptions: i) LK_s ranges for different textural classes were estimated from ROSETTA-predicted K_s values (see Table 3 in Paper III), which considered the standard deviation in ROSETTA predictions and the results of Paper I; and ii) drain spacing ranges in the stream baseflow

DRAINMOD simulation were based on the distance between the two branches of the Kleva river. A log-normal distribution function was used for LK_s, according to previous studies which indicated log-normal distribution for K_s (Tietje & Hennings, 1996; Giménez *et al.*, 1999), whereas a uniform distribution was chosen for DS. When there is little prior knowledge about a parameter, such as K_{c1} and K_{c2}, Beven & Binley (1992) recommend using a uniform parameter distribution with a wide range, which can be refined by comparison to the predicted response for defining a suitable reference prior distribution. A simple random Monte Carlo sampling was performed using uniform or log-normal distributions with 100 parameter sets simulated during Period 1 to Period 3 (calibration period).

Procedure for using likelihood weights in uncertainty estimation

The E values were renormalised such that the sum of all the E values was equal to 1, resulting in a distribution function for the parameter sets. To calculate a cumulative distribution of the predictions, the predicted values from each sample model run during a period were ranked in order of magnitude, using the likelihood weights associated with each simulation. For the present study, the 5% and 95% percentiles of the cumulative likelihood distribution were chosen as the uncertainty limits of the predictions. The 50% percentile was used as a measure of modal behaviour, which was compared with observed discharge and NO_3-N load values.

Procedure for updating likelihood weights recursively as new data become available

The likelihood weights associated with each model run and the predicted percentiles (5% and 95%) were updated as each new period of data was assimilated into the analysis from Period 1 to Period 3 (calibration period), using the Bayes equation.

Procedure for evaluating uncertainty such that the value of additional data can be assessed

The posterior likelihood distribution determined after Bayesian updating was used to validate Arc Hydro-DRAINMOD by comparison with observed data that were not used in the likelihood updating. This was done for Period 4 to Period 6 using the posterior likelihood distribution calculated for Period 1 to Period 3. In model calibration/validation, monthly observed and predicted percentile (5% and 95%) discharge and NO_3-N loads were compared by calculating the accumulated deviation (E_d). This statistical measure determines the percentage when the 5% and 95% model-simulated percentiles bracket the observations, which was adapted from the acceptability variables proposed by Thorndahl *et al.* (2008), given by:

$$E_{d,p} = \frac{\sum_{i=1}^{n} S_{i,p} - \sum_{i=1}^{n} O_i}{\sum_{i=1}^{n} O_i} \qquad \text{(Eq. 9)}$$

where O_i is the individual observed value at time i, $S_{i,p}$ is the individual simulated value at time i, p is the quantile (5% or 95%) and n is the number of paired observed-simulated values. The value of $E_{d,5\%}$ should be negative for a model, showing that the prediction is less than the observation and that overprediction is prevented. Correspondingly, $E_{d,95\%}$ should be positive for a model, showing that the prediction is larger than the observation and that underprediction is prevented.

4.3.5 Sensitivity analysis

In Paper IV, SA was carried out to identify parameters with great impact on NO_3-N load predictions. The GLUE results for all three parameters selected in the Monte Carlo simulations were used. In this study, the sensitivity analysis was performed by comparison of the cumulative distribution for the final behavioural simulations after all Bayesian updatings of likelihood weights and non-behavioural simulations. The parameters that showed a strong deviation between behavioural and non-behavioural cumulative distributions across the same parameter range can be considered the most sensitive. In contrast, parameters that were uniformly distributed were considered less sensitive to changes in parameter values.

In addition, the non-parametric Kolmogorov-Smirnoff d statistic (d_{K-S}) for the differences between behavioural and non-behavioural cumulative distributions was used as a relative measure of sensitivity (Beven, 2008).

5 Results and discussion

The results of running the DRAINMOD hydrological model with ROSETTA-estimated soil hydraulic properties at field scale are presented and evaluated in section 5.1 and those from modelling water discharge and NO_3-N load at field scale in section 5.2. Arc Hydro-DRAINMOD is evaluated as regards predicting discharge and NO_3-N loads at watershed scale in section 5.3 and 5.4, respectively. Results of the GLUE methodology are presented in sections 5.3 and 5.4 and some applications of the Arc-Hydro framework in section 5.5.

5.1 DRAINMOD estimation of drain outflow from agricultural fields using ROSETTA inputs (Paper I)

Results for the conventional drainage plot (CD) and for the controlled drainage plots (CWT1 and CWT2) are shown in Table 6. There was good agreement between observed and simulated monthly drainage outflows when the E' values indicated satisfactory agreement in CD ($E' \geq 0.62$), good agreement in CWT1 ($E' \geq 0.72$) and very good agreement in CWT2 ($E' \geq 0.79$). It is important to note that the H1 dataset, which estimated K_s from texture class, showed good agreement in all plots ($E' \geq 0.69$). These results suggest that ROSETTA-estimated K_s values from texture class can be used in DRAINMOD to simulate drainage outflows as accurately as measured K_s values (H0).

The ROSETTA-estimated K_s values caused the greatest deviation in simulated drainage outflow (*D*) for the three plots studied, as they showed the highest percent-normalised error (*NE*) (see Figure 2 in Paper I). In the CD plot, *D* values simulated with the H1-H4 datasets were higher than those simulated with the laboratory-measured K_s value (H0), with *NE* ranging from 11 to 12%. In CWT1 and CWT2, errors in predicted *D* were less than 2% with the one exception of the H3 dataset simulating *D* in CWT2 (*NE*=15%). In contrast, DRAINMOD showed a few errors in simulated infiltration (*F*) and evapotranspiration (*ET*) when ROSETTA-estimated K_s values were used. In *F*, *NE* values were less than 1% and most of the rainfall was predicted to infiltrate for all datasets due to the high K_s values in the coarse-textured soil profile. In most cases, *ET* values predicted with the ROSETTA-estimated K_s for the Gärds Köpinge soil were similar to those simulated with laboratory-measured K_s values, which showed *NE* values lower than 3%.

Table 6. *Observed and simulated overall drain outflow for conventional drainage plot (CD) and controlled drainage plots (CWT1 and CWT2) using five soil datasets (H0, H1, H2, H3 and H4)*

Plot	Observed (cm)	Simulated drain outflow (cm) using different datasets[a]/E'[b]				
		H0	H1	H2	H3	H4
CD	52.3	44.4/0.74	49.3/0.69	49.2/0.68	49.3/0.69	49.7/0.62
CWT1	23.4	25.5/0.73	25.9/0.72	26.0/0.72	25.9/0.73	25.4/0.74
CWT2	15.6	15.4/0.85	15.1/0.83	15.5/0.83	12.9/0.79	15.6/0.86

[a] H0: Laboratory-measured K_s; H1: ROSETTA-estimated K_s from texture class; H2: ROSETTA-estimated K_s from soil texture; H3: ROSETTA-estimated K_s from soil texture and ρb; H4: ROSETTA-estimated K_s from soil texture, ρb, θ_{33kPa} and $\theta_{1500kPa}$

[b] E' is the modified modelling efficiency comparing observed and simulated monthly values

5.2 DRAINMOD-N II estimation of drain outflow and nitrate loads from agricultural fields (Paper II)

5.2.1 Simulated drain outflow and snow cover

The drain flow pattern was well represented by the model in the three plots during the study period, when the model simulated most of the drainage outflows peaks in all plots during intensive events in autumn and early spring. Statistical comparisons between simulated and observed monthly drain outflows showed very good agreement for all plots, with the best agreement in calibration plot (CD) (Table 7).

In the calibration plot (CD), some differences were found for the autumn season in all periods of measurement, especially during high intensity precipitation events, and for the spring season during Period 1 and Period 2, when the model underpredicted observed drain outflows. In the CWT validation plots, there was no clear pattern of overprediction or underprediction of drainage outflows during the study period.

Table 7. *Observed and simulated overall drain outflow and NO_3-N loads for conventional drainage (CD) and controlled drainage (CWT1 and CWT2) plots*

Plot	Drain outflow			NO_3-N load		
	Observed	Simulated	*E* [a]	Observed	Simulated	*E* [a]
	—— cm ——			—— kg NO_3-N ha^{-1} ——		
CD	53.6	51.6	0.95	12.2	10.7	0.89
CWT1	29.4	33.3	0.84	10.6	9.4	0.55
CWT2	17.1	13.2	0.90	8.1	8.2	0.49

[a] *E* is the modelling efficiency comparing observed and simulated monthly values

At the experimental site, predicted and measured snowfall events were also in good agreement, as the model predicted 12 of 14 snow events and predicted snow cover on 82% of the measured days.

5.2.2 Simulated nitrate loads

Nitrate concentrations in drain outflows were strongly dependent on outflow rates in the three plots, when most of the monthly NO_3-N loads were recorded during intensive drainage outflow events in autumn and early spring. Similarly, in calibration plot CD the model correctly predicted the monthly pattern of drain outflows and its correlated NO_3-N loads. Thus for CD the *E* value of 0.89 indicated that observed and simulated monthly NO_3-N loads in subsurface drains were in very good agreement (Table 7). Only during October-March in Period 2 were observed NO_3-N loads not correctly predicted by the model, when it might have predicted less N mineralisation during the decomposition of pig slurry. In contrast to the CD, the *E* values of 0.55 and 0.49 in the respective CWT validation plots, were barely within the satisfactory range. In these plots, larger errors in predicting monthly NO_3-N drainage losses can be attributed to errors in prediction of N dynamics during the winter and early spring periods, when the model might have predicted much denitrification, leaving less mineral N susceptible to leaching in the profile.

5.2.3 Simulated nitrogen processes in soil

Table 8 shows a summary of N processes predicted by DRAINMOD-N for conventional drainage (CD) and controlled drainage (CWT) plots in the Gärds Köpinge field experiment in south-east Sweden. A comparison of N processes predicted by DRAINMOD-N and literature range values for Sweden (Johnsson *et al.*, 1987; Paustian *et al.*, 1990; Torstensson & Aronsson, 2000; Delin & Lindén, 2002) can be found in Table 14 in Paper II.

Table 8. *Annual average rates of net N mineralisation, nitrification, N plant uptake, denitrification, volatilisation and N wet deposition loads predicted by DRAINMOD-N II for the Gärds Köpinge field experiment in south-east Sweden*

Plot	Net mineralisation	Nitrifica-tion	Denitrifica-tion	Volatilisa-tion	Wet deposition
	kg N ha^{-1}				
CD	16.9	15.8	10.5	2.7	6.1
CWT1	53.0	35.9	11.1	2.9	6.1
CWT2	72.9	62.7	17.4	1.4	6.1

The predicted mean annual net mineralisation varied from 17 to 73 kg N ha^{-1} and showed large variations between periods. Unlike CD, CWT increased net mineralisation, probably due to the higher soil moisture content enhancing mineralisation in CWT plots during the summer period. This is consistent with the simulated groundwater level in CWT plots often ranging from 90 to 60 cm below the soil surface during the summer period, a groundwater level that was generally much higher than for CD.

Simulated nitrification was enhanced during the summer period, when temperature and moisture levels, which enhanced mineralisation, were also favourable for conversion of NH_4^+ to NO_3^-. In comparison to CWT plots, the mean annual simulated rate of nitrification was 56-75% smaller in CD. The soil moisture factor affecting mineralisation as discussed in the previous paragraph is also pertinent here. It is possible that in CD, nitrification processes declined during summer due to the lower soil moisture level than CWT. Consequently, CWT demonstrated higher measured NO_3-N content in the soil profile (0-90 cm) than CD, with significant differences in means of NO_3-N between plots CD and CWT2 (see Table 13 in Paper II).

Simulated rate of denitrification varied from 11 to 17 kg N ha^{-1} yr^{-1}, which appears reasonable compared with values reported at other sites in Sweden (Johnsson *et al.*, 1987; Paustian *et al.*, 1990; Torstensson & Aronsson, 2000). The effect of increasing the degree of waterlogging on denitrification was shown in CWT plots, where mean annual simulated rate of denitrification was 6% and 66% higher in CWT1 and CWT1 plots, respectively, than in CD. However, measurements of denitrification values would be necessary to confirm this trend. Denitrification rates appeared to be regulated by climate factors, such as amount and distribution of rainfall. For example, in Period 2, the period with the lowest precipitation between January and June (189 mm), the model did not predict gaseous N losses by denitrification in any plots.

The mean annual simulated volatilisation ranged from 1 to 3 kg N ha^{-1}, and was favoured by the high soil pH value at the site (7.5). In Period 1, all plots had the highest losses through volatilisation, which had its peak in April after application of NH_3-forming pig slurry.

Simulated wet deposition loads of NO_3-N and NH_4-N values were in agreement with those observed by the Swedish Environmental Research Institute in the county of Skåne (Liljergren, 2004).

5.3 Arc Hydro-DRAINMOD estimation of watershed discharge (Paper III)

5.3.1 Calibration, validation and uncertainty estimation

The temporal trend and magnitude of observed discharge at the watershed outlet were well predicted by Arc Hydro-DRAINMOD during the study period, when GLUE estimates showed good agreement with observed monthly discharge. The framework was capable of correctly predicting the highly seasonal discharge pattern of the Kleva river watershed, which had a phase of high discharge during winter and spring and a phase of low discharge during summer and autumn.

The likelihood threshold of acceptability $E \geq 0.6$ included a sufficient sample of model to form a meaningful cumulative weighted distribution of predictions. Thus, after all Bayesian updatings of likelihood weights during the calibration period, 68% of the simulations were retained as behavioural ($E \geq 0.6$).

In the calibration and validation periods, the uncertainty bands (5% and 95%) included a high percentage of the monthly observed values, about 88% and 75% respectively, showing good agreement between the GLUE estimates and measured monthly discharge (see Figures 3 and 4 in Paper III). Similarly, the overall accumulated deviation (E_d) of discharge volume indicated that neither overprediction nor underprediction occurred during the calibration period (see Table 7 in Paper III).

5.3.2 Simulated snow cover

At the experimental site, predicted and measured snowfall events were in good agreement, since the model predicted 14 of 17 snow events and predicted snow cover on 95% of the measured days. Similarly, Wesström (2002) and Paper II showed that DRAINMOD successfully simulated snow cover under the cold conditions of southern Sweden.

Some discrepancies in snow accumulation and snowmelt predictions were found in a mild winter in Period 5. This can also be observed in

Figure 4 in Paper III, where the measured discharge values were below the uncertainty bands during January-March in Period 5.

5.4 Arc Hydro-DRAINMOD estimation of nitrate loads from an agricultural watershed (Paper IV)

5.4.1 Calibration, validation and uncertainty estimation

Nitrate loads in the watershed were strongly dependent on discharge rates during the study period, with the highest NO_3-N concentrations recorded during intensive drainage outflow events in winter and spring (see Figure 2 in Paper IV). Similarly, the framework correctly predicted the monthly pattern of discharge and its correlated NO_3-N loads, when GLUE estimates showed good agreement with observed monthly NO_3-N loads.

The likelihood threshold of acceptability $E \geq 0.3$ included a sufficient sample of model to form a meaningful cumulative weighted distribution of predictions. Thus, after all Bayesian updatings of likelihood weights during the calibration period, 60% of the simulations were retained as behavioural ($E \geq 0.3$).

In the calibration and validation periods, the uncertainty bands (5% and 95%) included a high percentage of the monthly observed values, about 71% and 67% respectively, showing good agreement between the GLUE estimates and measured monthly NO_3-N load (see Figures 3 and 4 in Paper IV). Similarly, the overall accumulated deviation (E_d) of NO_3-N load indicated that neither overprediction nor underprediction occurred during the calibration period (see Table 6 in Paper IV).

5.4.2 Sensitivity analysis

Both visual and statistical analysis showed that the watershed boundary for stream baseflow simulation (DS) and the decay coefficient 1 (k_{c1}) were the most sensitive parameters (see Figure 5 in Paper IV). These parameters represent stream baseflow and N removal in the stream network, which were probably the most poorly known processes during this framework evaluation because measurements were outside the scope of this study and few literature data were available for comparison with framework-predicted values.

5.5 Simulating hydrological and nitrogen processes in the watershed

The 50% GLUE estimate results of water discharge and NO_3-N loads for the Kleva river watershed were used to evaluate the performance of the framework at different time scales and to show some applications of Arc Hydro-DRAINMOD.

Very good agreement was found between observed and 50% GLUE estimate values at a monthly time scale. Simulated results of monthly discharge and NO_3-N loads for the Kleva river watershed during Period 1 to Period 6 showed E values higher than 0.75 and differences less than 7% and 14% in overall discharge and NO_3-N load, respectively (Table 9).

Table 9. *Comparison of observed and simulated 50% GLUE estimate discharge and NO_3-N loads during Periods 1-6*

Value	Discharge		NO_3-N load	
	(x 10^3 m^3) [a]	E [b]	(ton) [a]	E [b]
50%	3447	0.84	18.4	0.76
Observed	3218		21.4	

[a] Overall discharge and NO_3-N loads during Periods 1-6

[b] E is the modelling efficiency comparing observed and simulated monthly values.

Major discrepancies in monthly discharge predictions were found in January-March in Period 5, when DRAINMOD overpredicted discharge due to errors in snow accumulation and snowmelt in this mild winter (see outliers in Figure 3).

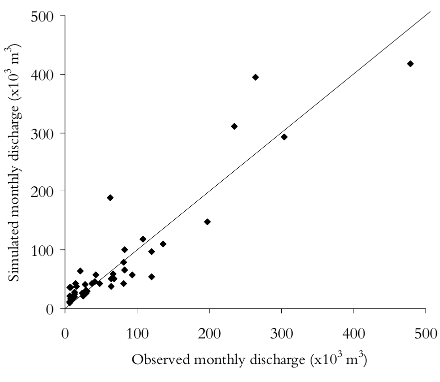

Figure 3. Scatter diagram comparing observed and 50% GLUE estimate-predicted monthly discharge from Period 1 to Period 6.

Major discrepancies in predicting monthly NO_3-N loads were found in Period 3 and January-March in Period 5 (see outliers in Figure 4), which could be attributable to errors in predicting watershed discharge volumes. Other possible explanations are that the framework might have predicted lower NO_3-N loads from the stream baseflow or much denitrification in the stream network. However, these processes were not measured, so it was not possible to directly test the accuracy of framework prediction of these processes.

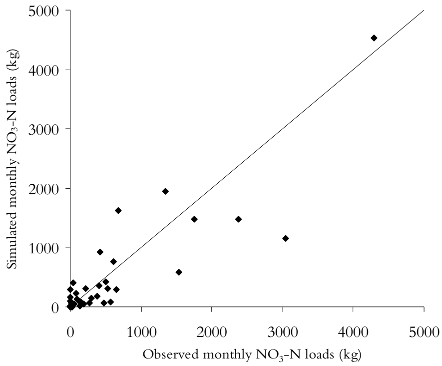

Figure 4. Scatter diagram comparing observed and 50% GLUE estimate-predicted monthly NO_3-N loads from Period 1 to Period 6.

In contrast to monthly simulations, on a daily time scale the 50% GLUE estimate simulations showed some longer response times for peaks (see Figure 5 in Paper III), which suggests that the assumption of constant water flow velocity in the stream network with a time lag of one day needs to be revised if the framework is to be used for daily time step simulations.

Arc Hydro-DRAINMOD also proved capable of evaluating land use management practices as regards the spatial variability within the watershed. For instance, an application of the framework can be to consider the contribution from fields with different soil types and stream baseflow to discharge and NO_3-N loads. For example, Figure 5 shows that the coarse-textured fields (sand, loamy sand, and sandy loam), comprising about 75% of the soil type in the watershed area, accounted for 40% of the outflow to watershed discharge and 67% of the NO_3-N load to the watershed. Therefore, coarse-textured fields were identified as the main source of NO_3-N loads in the Kleva river watershed. Although organic soils represented only 9% of the soils in the watershed and 4% of the outflow to watershed discharge, they accounted for 24% of the NO_3-N load to watershed NO_3-N load received and were the second most important source of NO_3-N loads in the Kleva river watershed. In contrast, silty loam soils occupied 16% of the watershed area and accounted for 14% of the outflow to watershed discharge, but delivered only 1% of the NO_3-N load to the watershed. These results suggest that best management practices (BMPs) to reduce NO_3-N loads within the watershed should be concentrated to fields with coarse-textured or organic soils, which were shown to be more prone to nitrate losses.

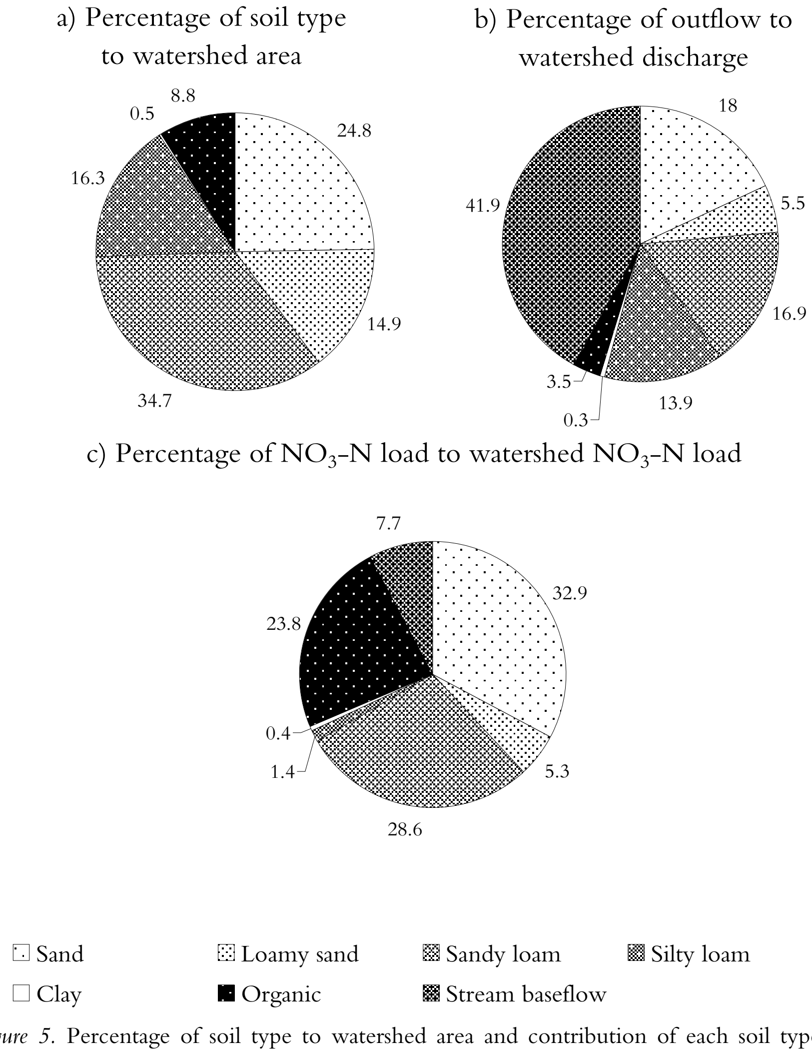

Figure 5. Percentage of soil type to watershed area and contribution of each soil type and stream baseflow to watershed discharge and NO_3-N load received at the watershed outlet during Period 1 to Period 6 using the 50% percentile GLUE estimate

Although field outflow was the major source of outflow to the watershed discharge (58%) during the study period, there was also an important contribution from stream baseflow (42%). However, most of the NO_3-N load received at the watershed outlet was quickly delivered from fields (92%), with a slow response from the stream baseflow (8%).

Results from the 50% percentile GLUE estimate also showed that 25% of the overall NO_3-N load was removed in the stream network and 75% of the overall NO_3-N load passed through the watershed outlet. The simulated rate of N removal (due to denitrification) on an overall basis appears reasonable with respect to previous estimates (Saunders & Kalff, 2001; Seitzinger *et al.*, 2002; Lepistö *et al.*, 2006; Birgand *et al.*, 2007; Appelboom *et al.*, 2008). However, measurements of N removal mechanisms and values from the network of the Kleva river would be necessary to confirm this trend.

Other applications of Arc Hydro-DRAINMOD include evaluation of the effects of different crops on the water balance for each field (see Table 10 in Paper III) and estimation of the effects of different crop rotations and management on the N balance in each field (see Table 9 in Paper IV).

6 Conclusions

In relation to the initial objectives formulated it was concluded that:

- There was good agreement between observed and DRAINMOD-simulated drainage rates using K_s values estimated by PTFs. This demonstrates the feasibility of running DRAINMOD with estimated K_s values by PTFs.

- There was good agreement between observed and DRAINMOD-simulated monthly drain outflows and DRAINMOD-N II-simulated NO_3-N loads in drained agricultural fields. The results presented here indicate that these models can be used to predict discharge and NO_3-N loads from drained land at field scale in southern Sweden.

- The temporal trend and magnitude of monthly measured discharge were well predicted by Arc Hydro-DRAINMOD, indicating that Arc Hydro-DRAINMOD can be an effective tool for describing hydrological processes at watershed scale in southern Sweden.

- Although the performance of Arc Hydro-DRAINMOD on a daily basis showed promising results, the time lag of the watershed response needs to be revised if the framework is to be used for daily time step simulations of discharge.

- The temporal trend and magnitude of monthly measured NO_3-N loads were well predicted by Arc Hydro-DRAINMOD, demonstrating that Arc Hydro-DRAINMOD can be used to predict NO_3-N loads at watershed scale in southern Sweden.

- In prediction of NO_3-N loads at watershed-scale, sensitivity analyses showed that the distance between the river and the watershed boundary (DS) and the decay coefficient 1 (k_{c1}) were the most sensitive parameters. DS affects the NO_3-N loads from the stream baseflow, while k_{c1} affected N removal in the stream network.

- The GLUE methodology proved to be an applicable and formal basis for uncertainty estimation of discharge and NO_3-N load predictions.

- The good agreement in Arc Hydro-DRAINMOD predictions showed that with a distributed modelling approach it is possible to aggregate the results of field-scale simulations to estimate hydrology and water quality responses at watershed scale for artificially drained land. Using fields as the modelling unit gave the best degree of accounting for spatial and temporal variations in simulation of hydrology and nitrogen processes in a watershed in southern Sweden.

- These models can contribute to evaluate the combined effects of soil type and crop rotation in order to improve water use efficiency in watersheds and to evaluate best management practices (BMPs) to reduce NO_3-N loads within the watershed. For instance, BMPs may be prioritised in fields more prone to nitrate losses, such as fields with coarse-textured or organic soils.

7 Future research

The general agreement in predictions of water discharge and NO_3-N loads at field and watershed scale using this approach is encouraging. Initial experiences with DRAINMOD/DRAINMOD-N II at field scale and Arc Hydro-DRAINMOD at watershed scale show that these models are applicable for predicting discharge and NO_3-N loads from drained agricultural soils. This thesis identified the following areas where additional data would help to improve model performance:

- Measurements of denitrification that can be compared with DRAINMOD-N II-simulated denitrification rates. This could confirm whether errors in prediction of N dynamics during the winter and the early spring periods were due to errors in simulation of denitrification.

- Measurements of stream baseflow and N removal in the stream network, which were identified as the most sensitive factors in NO_3-N load predictions at watershed scale. Quantification of these processes could improve the accuracy of estimated water discharge and NO_3-N loads at watershed scale.

- Better characterisation of the travel time (time lag) of water and nitrate from the field edge to the watershed outlet, where data on additional parameters such as flow velocity and water column depth could improve daily predictions.

However, these processes represent a challenge in hydrological modelling due to the difficulty in obtaining measured data. Although accurate characterisation of these processes may help to reduce uncertainty, it is unlikely that all uncertainty in model predictions will disappear with the availability of more and better field measurements. Therefore, uncertainty analysis must be included in future model evaluations. This study showed the GLUE methodology to be an adequate procedure for uncertainty estimation. However, additional work is still needed in the GLUE procedure to better define acceptability levels and requirements for a model to be considered behavioural, which will be considered in future framework evaluations.

Another topic that would help to improve model performance would be the development of PTFs from the Swedish soil database at the Division of Agricultural Hydrotechnics, SLU, which has a complete dataset of soil physical properties and associated soil hydraulic properties. Future Swedish PTFs could be included in Arc Hydro-DRAINMOD to refine the range of soil hydraulic property distributions used in the simulations.

Future applications of Arc Hydro-DRAINMOD could include evaluations of the effects of different water management strategies on conserving water and minimising nitrate loads in watersheds. For instance, controlled drainage and subirrigation systems could be included in fields with soils more prone to nitrate losses in order to reduce nitrate loads reaching the stream network in artificially drained watersheds.

On the other hand, Arc Hydro-DRAINMOD is still a complex system and there is a need to develop easier means for input data preparation to increase the framework applicability. To make this tool more user-friendly, future work should examine *e.g.* automatic parameterisation routines, a better interface between the models and GIS and automatic generation of graph and table outputs to demonstrate the framework's capabilities to potential model users.

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Special Appendix (see section 8 for sources)

DRAINMOD-N II input parameters for management and crop production

Table A1. *Potential yield (grain/seed), plant shoot and root dry matter values of peas, potatoes, ryegrass, barley, sugarbeet and wheat reported in the literature.*

Crop	Grain /seed	Shoot	Root	Reference
	—— kg DM ha^{-1} ——			
Barley	5700	–	–	Gärds Köpinge (Wesström, 2006)
	4100	–	–	Gärds Köpinge (Wesström, 2006)
	4730	–	–	Kalmar county (Jordbruksverket, 2003, 2004a, 2004b, 2005, 2006 & 2007).
Peas	2670	–	–	Kalmar county (Jordbruksverket, 2003, 2004a, 2004b, 2005, 2006 & 2007).
Potatoes	–	–	–	Vos (1997)
	–	–	15400	Gärds Köpinge (Wesström, 2006)
Ryegrass	–	3870	–	Kalmar county (Jordbruksverket, 2003, 2004a, 2004b, 2005, 2006 & 2007)

Continuation Table A1

Sugarbeet	–	–	19000	Gärds Köpinge (Wesström, 2006)
Wheat	5400			Gärds Köpinge (Wesström, 2006)
	6740			Kalmar county (Jordbruksverket, 2003, 2004a, 2004b, 2005, 2006 & 2007)

Table A2. *Values for harvest index (HI), root/shoot ratio (rsr), and grain/seed nitrogen content (*N*) of peas, potatoes, ryegrass, barley, sugarbeet and wheat reported in the literature.*

Crop	*HI*	*rsr*	N	Reference
			%	
Barley				
	–	0.08	–	Kirby & Rackham (1971)
	0.50	–		Prince *et al.* (2001)
	–	–	1.58	Wesström (2006)
	0.50	0.08	1.58	Average
Peas				
	–	0.38	–	Bandyopadhyay *et al.* (1996)
	0.41	–	–	Chandra & Polisetty (1998)
	0.51	–	–	Lecoeur & Sinclair (2001)
	–	–	4.53	Lhuillier-Soundélé *et al.* (1999)
	0.46	0.38	4.53	Average
Potatoes				
	0.07	–	–	Calculated using: a seed yield of 145 kg ha^{-1} (Roy *et al.*, 2007); and shoot dry matter of 2 ton ha^{-1} (Vos, 1997)
	–	7.61	–	Calculated using: a seed yield of 145 kg ha^{-1} (Roy *et al.*, 2007); root dry matter of 15 ton ha^{-1} (Wesström, 2006); and harvest index of 0.07
	–	–	0.41	Roy *et al.* (2007)
	0.07	7.61	0.41	Average
Ryegrass				
	0.15	–	–	Calculated using: a seed yield of 520 kg ha^{-1} (Svensson & Boelt, 1997); and shoot dry matter of 4 ton ha^{-1} (Jordbruksverket, 2007).
	–	0.15	–	Cullen *et al.* (2006)
	–	–	2.00	Ene & Bean (1975)
	0.15	0.15	2.00	Average

Continuation Table A2

Crop	*HI*	*rsr*	N	Reference
			%	
Sugarbeet				
	0.27	–	–	Calculated using: a seed yield of 1100 kg ha^{-1} (Kaw & Mir, 1975); and shoot dry matter of 3 ton ha^{-1} (Wesström, 2006)
	–	4.67	–	Calculated using: a seed yield of 1100 kg ha^{-1} (Kaw & Mir, 1975); root dry matter of 19 ton ha^{-1} (Wesström, 2006); and harvest index of 0.27
	–	–	2.00	Longden (1970)
	0.27	4.67	2.00	Average
Wheat				
	0.46	0.10	–	Youssef *et al.* (2006)
	–	–	2.37	Wesström (2006)
	0.46	0.10	2.37	Average

Table A3. *Values for shoot chemical composition of peas, potatoes, ryegrass, barley, sugarbeet and wheat reported in the literature.*

Crop	N	C	Lignin	Reference
	———	%	———	
Barley				
	0.59	47.30	6.10	Henriksen & Breland (1999)
	0.59	47.30	6.10	Average
Peas				
	2.71	46.70	8.90	Jensen (1996)
	1.50	40.50	7.40	Kumar & Goh (2003)
	2.13	43.60	–	Lazarev & Maisyamova (2006)
	–	–	6.00	López *et al.* (2005)
	2.11	43.60	7.43	Average
Potatoes				
	4.90	35.28	8.40	Bending *et al.* (1998)
	2.60	45.70	6.50	Henriksen & Breland (1999)
	4.68	–	–	Warman & Havard (1998)
	4.06	40.49	7.45	Average
Ryegrass				
	3.40	35.70	4.60	Bending *et al.* (1998)
	1.81	46.00	1.40	Henriksen & Breland (1999)
	2.74	–	–	Thomsen (1993)
	3.45	41.45	3.00	Thorup-Kristensen (1994)
	1.75	–	–	Torstensson & Aronsson (2000)
	2.63	41.05	3.00	Average
Sugarbeet				
	–	26.23	4.20	Bending *et al.* (1998)
	2.30	–	–	Wesström (2006)
	2.30	26.23	4.20	Average
Wheat				
	0.73	–	–	Youssef (2003)
	–	41.50	5.70	Youssef *et al.* (2006)
	0.73	41.50	5.70	Average

Table A4. *Values for root chemical composition of peas, potatoes, ryegrass, barley, sugarbeet and wheat reported in the literature.*

Crop	N	C	Lignin	Reference
	—— % ——			
Barley				
	1.80	39.20	–	Schnürer & Rosswall (1987)
	–	–	23.10	Singh *et al.* (2007)
	1.80	39.20	23.10	Average
Peas				
	3.25	44.60	13.20	Jensen (1996)
	1.82	40.90	–	Lazarev & Maisyamova (2006)
	2.04	41.00	16.00	Soon & Arshad (2002)
	2.37	42.20	14.60	Average
Potatoes				
	1.4	–	–	Wesström (2006)
	1.4	–	–	Average
Ryegrass				
	2.20	36.60	7.90	Bending *et al.* (1998)
	0.96	–	–	Thomsen (1993)
	1.58	39.60	7.90	Average
Sugarbeet				
	0.76	–	–	Wesström (2006)
	0.76	–	–	Average
Wheat				
	0.86	–	–	Youssef (2003)
	–	36.50	9.50	Youssef *et al.* (2006)
	0.86	36.50	9.50	Average

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