INSTITUT FÜR HYDROLOGIE
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Distributed Solute Transport Modelling in the Fyrisån Catchment in Sweden

Diplomarbeit unter Leitung von Prof. Dr. Ch. Leibundgut

Freiburg i. Br., März 2005

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Koreferent: Dr. J. Lange

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How could drops of water know themselves to be a river?
Yet the river flows on

Antoine de Saint-Exupéry

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Sebastian Wrede

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Notations

%	Percent	
°C	Degree Celsius	
ϕ	Lumped effect of biochemical transformation	(mg d^{-1})
a	Year	
ActET	Actual evaporation	(mm d^{-1})
Al	Aluminium	
$ALPHA_{lake}$	Nonlinear weighting coefficient for lakes	
A_{mean}	Mean average cross sectional area of measuring section	(m^2)
a.s.l.	Above sea level	
$BETA_{agricul}$	Shape coefficient for agriculture	
$BETA_{forest}$	Shape coefficient for forest	
$BETA_{urban}$	Shape coefficient for urban	
$BETA_{wetland}$	Shape coefficient for wetland	
b_x	Distance from initial point to vertical x	(m)
$b_{(x-1)}$	Distance from initial point to preceding vertical	(m)
$b_{(x+1)}$	Distance from initial point to next vertical	(m)
c	Concentration	(quantity m^{-3})
c_i	Inflow concentration	(quantity m^{-3})
Ca	Calcium	
CFMAX	Degree-day factor	(mm °C d^{-1})
CFR	Refreezing coefficient	
CO_2	Carbon dioxide	
Corrected precip	Corrected solid precipitation	(mm d^{-1})
CWH	Water holding capacity	
d	Day	
D	Atmospheric deposition on open water bodies	
D8	Single-flow direction algorithm	
DEM	Digital elevation model	
d_i	Distance to gauging station	(m)
DIN	Dissolved inorganic nitrogen	
DMAX	Flow distribution length	
dN/dt	Nitrogen flux	(mg d^{-1})
DON	Dissolved organic nitrogen	
DPEAK	Flow distribution length to peak	
d_x	Depth of water at vertical x	(m)
EML	Environmental modelling language	
Eq.	Equation	
EU	European Union	
$FC_{agricul}$	Field capacity for agriculture	(mm)
FC_{forest}	Field capacity for forest	(mm)
FC_{urban}	Field capacity for urban	(mm)
$FC_{wetland}$	Field capacity for wetland	(mm)
Fe	Iron	
Fraction of lake	Fraction of lake according to sub-grid parameterisation	
Fraction of landuse	Fraction of land use according to sub-grid parameterisation	
GIS	Geographic information system	

GPS	Global-positioning system	
ha	Hectare	
$H_{LS\ agricul}$	Minimal storage capacity lower box agriculture	(mm d^{-1})
$H_{LS\ forest}$	Minimal storage capacity lower box forest	(mm d^{-1})
$H_{LS\ urban}$	Minimal storage capacity lower box urban	(mm d^{-1})
$H_{US\ agricul}$	Maximal storage capacity upper box agriculture	(mm d^{-1})
$H_{US\ forest}$	Maximal storage capacity upper box forest	(mm d^{-1})
$H_{US\ urban}$	Maximal storage capacity upper box urban	(mm d^{-1})
$H_{US\ wetland}$	Maximal storage capacity upper box wetland	(mm d^{-1})
i	Time step	
IAKS	Integrated Administrative Control System for agricultural EU subsidies	
InSoil	Input into soil routine	(mm d^{-1})
ISO	International Organisation for Standardisation	
k	Storage coefficient	(1 time $step^{-1}$)
k	Discharge correction factor	
K	Potassium	
$k_{Groundwater}$	Retention factor in groundwater	
Kjeld-N	Kjeldahl nitrogen	
k_{Lake}	Retention factor in lakes	
K_{lake}	Recession coefficient lake	(d^{-1})
$K_{LS\ agricul}$	Lower recession coefficient for agriculture	(d^{-1})
$K_{LS\ forest}$	Lower recession coefficient for forest	(d^{-1})
$K_{LS\ urban}$	Lower recession coefficient for urban	(d^{-1})
$K_{US\ agricul}$	Upper recession coefficient for agriculture	(d^{-1})
$K_{US\ forest}$	Upper recession coefficient for forest	(d^{-1})
$K_{US\ urban}$	Upper recession coefficient for urban	(d^{-1})
$K_{US\ wetland}$	Upper recession coefficient for wetland	(d^{-1})
$k_{Wetland}$	Retention factor in wetlands	
Lake_box	Storage in lake	(mm)
LDD	Local drain direction (network)	
LP	Reduction parameter of field capacity	
LS_box	Storage in lower zone	(mm)
LS_H	Lower storage threshold	
LS_K	Recession coefficient for lower zone	(d^{-1})
MATCH	Mesoscale Atmospheric and Chemistry (model)	
MAXBAS	Empirical HBV flow weighting parameter	
Mg	Magnesium	
Mn	Manganese	
n	Duration of simulation period	
N	Nitrogen	
N_2O	Nitrous oxide	
Na	Sodium	
NH_3	Ammonia	
NH_4^+	Ammonium	
NO	Nitrate monoxide	
NO_2^-	Nitrite	
NO_3^-	Nitrate	
O^{18}	Oxygen isotope	
Observed precip	Observed precipitation	(mm d^{-1})
P	Precipitation	(mm d^{-1})

PCRaster	Dynamic GIS Software	
PEAK	Flow distribution peak location	
$PERC_{agricul}$	Percolation from upper to lower box agriculture	(mm d^{-1})
$PERC_{forest}$	Percolation from upper to lower box forest	(mm d^{-1})
$PERC_{urban}$	Percolation from upper to lower box urban	(mm d^{-1})
PEST	Parameter ESTimation Software	
pH	Pondus hydrogenii or potentia hydrogenii	
P	Point source	
PO_4^{3-}	Phosphate	
PON	Particulate organic nitrogen	
PotET	Potential evaporation	(mm d^{-1})
q	Specific discharge	(m^3 s^{-1} km^{-2})
Q	Discharge	(m^3 s^{-1})
$Q_{i, obs}$	Observed runoff at time step i	(mm time $step^{-1}$)
$Q_{i, sim}$	Simulated runoff at time step i	(mm time $step^{-1}$)
Q_{in}	Runoff inflow	(mm d^{-1})
Q_Lake	Runoff at lake outlet	(mm d^{-1})
Q2_LS	Runoff component from lower zone	(mm d^{-1})
Q1_US	Runoff component from upper zone	(mm d^{-1})
$\overline{Q_{obs}}$	Mean observed runoff for the whole observation period	(mm time $step^{-1}$)
Q_{out}	Runoff outflow	(mm d^{-1})
$\overline{Q_{sim}}$	Mean simulated runoff for the whole observation period	(mm time $step^{-1}$)
r	Weighting coefficient of reciprocal distance	
R_{eff}	Model efficiency	
Refreezing melt water	Amount of melt water that refreezes	(mm d^{-1})
R_v	R_v criterion	
s	Second	
SFCF	Snowfall correction factor	
$SFCF_{diff}$	Snowfall correction factor for forest	
Si	Silicate	
SLU	Swedish University of Agricultural Science	
SMHI	Swedish Meteorological and Hydrological Institute	
Snowmelt	Melt water of snow	(mm d^{-1})
Snowpack	Water equivalent of snowpack	(mm d^{-1})
SoilMoisture	Actual soil moisture	(mm)
SRTM DEM	Digital Elevation Model derived from the Shuttle Radar Topography Mission	
SUrbanSplit	Urban split factor	
SVAT	Soil-Vegetation-Atmosphere-Transfer (scheme)	
t	Time	t
T	Mean daily air temperature	(°C d^{-1})
T_{10}	10-day-mean air temperature	(°C)
TAC^D	Tracer aided catchment model, distributed	
TDN	Total dissolved nitrogen	
TOC	Total organic carbon	
ToRunoffGeneration	Infiltration into the runoff generation routine as a fraction of the actual soil moisture	(mm d^{-1})
Tot-N	Total nitrogen	

Tot-P	Total phosphorus	
TRK	TRK project	
TT	Temperature threshold parameter	(°C d^{-1})
TT_{diff}	Temperature threshold parameter for forest	(°C)
UrbanSplit	Portion of sealed urban areas	(d^{-1})
US_box	Storage in upper zone	(mm)
US_H	Upper storage threshold	
US_K	Recession coefficient for upper zone	(d^{-1})
US_Perc	Percolation from upper storage	(d^{-1})
USGS	United States Geological Survey	
V	Water volume of response box, river or lake	(mm d^{-1})
V	Storage level	(mm)
V_0	Storage level at time t = 0	(mm)
V_E	Relative volume error	
v_{max}	Measured velocity of surface stream flow	(m s^{-1})
V(t)	Storage level at time t	(mm)
v_x	Mean velocity at vertical x	(m s^{-1})
w	Weight	
Water content	Water content of snow cover	(mm d^{-1})
WFD	Water Framework Directive	
WMO	World Meteorological Organisation	
z(x)	Interpolated value at location x_0	
$z(x_i)$	Measured value at gauging station	

Abstract

Eutrophication of inland and costal waters is a major environmental thread towards aquatic ecosystems and serious efforts are inevitable to reduce emissions and to achieve a better status of surface waters. Thus tools for quantification of nutrient flow and source apportionment are urgently needed for implementing national and international water quality guidelines. To facilitate an integrated management of water resources, it is essential to develop catchment models that are capable of simulating water quantity as well as quality. The main objective of this thesis was the development and evaluation of a distributed conceptual model that enables nitrogen transport based on an underlying hydrological model at the catchment-scale. The applicability of the model was demonstrated in the mesoscale low land Fyrisån catchment in Sweden.

A fundamental prerequisite for a successful model application is the availability of input data. Comprehensive data sets were collected, processed, and allocated in a central data base to make further model testing possible. Additionally a synoptic sampling campaign was carried out to complete the available data base with information about spatial chemical and hydrological parameters. The obtained data gave insight in spatial nitrogen concentrations and runoff patterns. Furthermore the synoptic sampling campaign provided a valuable data set for subsequent intensive evaluation of the hydrological and the solute transport models.

Model development and testing was done step-wise and separately for the hydrological and solute transport model. Starting point for the development of the hydrological model were the model concepts of TAC^D and HBV. Key features obtained from both model concepts contained the structure of the HBV model concept with its sequentially linked routines and the distribution and specially designed land use based runoff generation routine of the TAC^D model. To account for distinct landscape features of the low land Fyrisån catchment, the hydrological model was additionally equipped with a sub-grid parameterisation scheme and flow and lake distribution routines. Calibration of the model was achieved against daily runoff data at two gauging stations by the automated parameter estimator PEST. An intensive test procedure was carried out that involved split-sample test, proxy-basin test, evaluation against synoptic measurements, and the comparison against a simple lumped HBV model. Besides an overall good model performance, the evaluation revealed problems of the hydrological model to capture spatial runoff patterns adequately. Moreover the performance of the simpler lumped HBV model was equal to slight superior to the distributed model.

The application of the solute transport model was guided by concepts of HBV-N and TAC^D. A model routine for conservative routing of solute was adopted from the TAC^D model, while retention functions were obtained from the HBV-N model concept. The nutrient transport model was coupled to the underling hydrological model and calibration of the nitrogen model to observed monthly nitrogen concentrations revealed problems of the model to capture the seasonally and spatial concentration pattern of total nitrogen correctly. However, simulation of gross and net load were in line with other model results in the Fyrisån catchment. Although the intensive testing revealed problems of both, the hydrological and the transport model, the overall model performance was considered to be on the same level with other nutrient transport models, since most of the identified problems were only discovered by detailed and critical model testing or could be attributed to the high uncertainty involved in nitrogen transport modelling.

The presented version of the nitrogen transport model can be regarded as a framework for continuing research and development and the created data base encourages further model applications and comparisons in the Fyrisån catchment.

Keywords:

Distributed HBV model
Distributed nitrogen transport modelling
Sub-grid parameterisation scheme
Flow and lake routing
Synoptic sampling
Fyrisån catchment
Nordic hydrology

Zusammenfassung

Die Eutrophierung von Binnen- und Küstengewässern führt zu einer zunehmenden Gefährdung von terrestrischen Oberflächengewässern, so dass zukünftig einschneidende und effiziente Maßnahmen zur Reduzierung der Emissionen unvermeidbar werden, um eine Verbesserung der Oberflächengewässerqualität zu erreichen. Mittel zur Quantifizierung von Nährstofffrachten, sowie Kenntnisse über Anteile verschiedener Emissionen sind dringend notwendig, um nationale und internationale Wasserqualitätsrichtlinien umzusetzen. Ein integriertes Management von Wasserressourcen erfordert daher insbesondere auch die Entwicklung von Modellsystemen, welche in der Lage sind sowohl Wasserqualität als auch Wasserquantität zu simulieren. Hauptziel dieser Arbeit war die Entwicklung und Evaluierung eines distribuierten, konzeptionellen Modells, welches die Simulation von Stickstofftransport auf der Grundlage eines hydrologischen Modells in der Einzugsgebietsskale ermöglicht. Die Anwendbarkeit dieses Modells wurde in dem mesoskaligen Fyrisån Einzugsgebiet in Schweden demonstriert.

Die verfügbare Datenbasis in einem Einzugsgebiet hat einen maßgeblichen Einfluss auf die Art und Qualität der Modellanwendung. Ausgangspunkt der Modellanwendung war die Sammlung und Aufarbeitung umfangreiche Datensätze und deren Bereitstellung in einer zentralen Datenbank. Zusätzlich wurde eine flächendeckende synoptische Stichtagsbeprobung durchgeführt. Die so gewonnenen hydrologischen und chemischen Parameter, erlaubten Einblicke in die räumlichen Muster von Stickstoffskonzentrationen und Abflusswerten im Einzugsgebiet und ermöglichten eine intensive Evaluierung des hydrologischen Modells, als auch des Transportmodells.

Modellentwicklung und -tests wurden schrittweise für beide Modelle durchgeführt. Ausgangspunkt für die Entwicklung des hydrologischen Modells bildeten die Konzepte von TAC^D und HBV. Während vom HBV Modell die generelle Modellstruktur und Modellroutinen als Grundlage verwendet wurden, lieferte das TAC^D Modell die räumliche Distribuierung, als auch das räumliche differenzierte Abflussbildungsmodul. Um den naturräumlichen Gegebenheiten des Gebietes besser zu entsprechen, wurde zudem ein zusätzlicher sub-grid Parametrisierungsansatz verwendet und ein einfaches Fluss-Routing und Seenmodul implementiert. Anschließend an die hydrologische Modellentwicklung wurde das Modell mithilfe der automatischen Kalibrierungsroutine PEST an verfügbaren täglichen Abflussdaten an zwei Pegeln im Gebiet optimiert und eine intensive Modellevaluierung durchgeführt. Diese beinhaltete unter anderem: split-sample tests, proxy-basin tests, einen Modellvergleich mit einem einfachen lumped HBV Modell und einen Vergleich mit den gewonnenen synoptischen Messdaten. Neben einer akzeptablen Gesamtperformance, offenbarte das Ergebnis Schwächen des Modells räumliche Abflussmuster zu erfassen und zu reproduzieren. Ferner war es nicht möglich, bessere Modellergebnisse als mit dem einfachen HBV Modell zu erzielen.

Die Anwendung des Transportmodells wurde ebenfalls an Konzepte aus dem HBV-N Modell und TAC^D Modell angelehnt. Während vom TAC^D Model die grundlegende Struktur für den konservativen Stofftransport übernommen wurde, ermöglichten vom HBV-N Modell entnommene Funktionen die Beschreibung von Stickstoff-Retention.

In einem nächsten Schritt wurde das Transportmodell an das zugrunde liegende hydrologische Modell gekoppelt und eine Kalibrierung des Stofftransportmodells erfolgte gegen monatliche Zeitreihen gemessener Stickstoffkonzentrationen. Die Ergebnisse offenbarten Probleme des Modells, saisonale Schwankungen angemessen zu reproduzieren, sowie analog zum hydrologischen Modell, räumliche Muster korrekt wiederzugeben. Dagegen entsprach die Simulation der Gesamtfracht und Retention im Gebiet den Ergebnissen früherer Studien.

Insgesamt wurde die Modellperformance als vergleichbar zu anderen Modellen eingestuft, wobei die Schwächen des Modells auf die großen bestehenden Modell- und Datenunsicherheiten, als auch auf die sehr intensive Evaluierungs- und Testprozeduren zurückgeführt werden konnten.

Damit kann die vorliegende Version des Transportmodells als Grundlage für eine weitergehende Entwicklung und Untersuchung von Stickstofffrachten im Untersuchungsgebiet gesehen werden. Die geschaffene Datenbank erleichtert dabei die Durchführung und den Vergleich weiterer Modellanwendungen im Fyrisån Einzugsgebiet.

1. Introduction

Eutrophication of surface water is considered as one of the major environmental threats towards European aquatic ecosystems. Eutrophication has been an environmental problem ever since the beginning of the industrial era, and it is strongly associated with urbanisation and efficient industrial and agricultural production. The effect of eutrophication is high production of plankton algae leading to oxygen deficiency which in turn can lead to fish death, reduced biological diversity, bottom death, and toxic substances in the water. The prevailing opinion is that the eutrophication problem is caused by high nitrogen and phosphorus loads. For instance, the loads of nitrogen and phosphorus to the Baltic Sea from rivers largely exceeds the input from other sources such as atmospheric deposition and direct emission from point sources (KRONVANG ET AL. 1993; STALNACKE ET AL. 1999) and are thereby primarily responsible for eutrophication problems in this region. Thus tools for quantifying nutrient flows and source apportionment are urgently needed for implementing national and international environmental regulations such as the EU Water Framework Directive (WFD). These guidelines demand that all waters within the Union shall be brought to a “good status” and shall be managed in a sustainable way by 2015 (EC 2002). Hence it is essential to develop catchment models that are able to simulate water quantity as well as quality for an integrated management approach protecting water resources. Many solute transport models were developed in recent years ranging from relatively simple empirical models to physically based models (e.g. SHETRAN: BIRKINSHAW & EWEN 2000; ANIMO: RIJTEMA & KROES 1991; INCA: WHITEHEAD et al. 1998) which are able to simulate water and solute transport with high temporal and spatial resolution. While the latter can only be applied to highly instrumented small-scale test sites (e.g. ANIMO: RIJTEMA & KROES 1991), the advantage of simpler models is that the limited data requirement allows also an application to large scales, i.e. the catchment-scale (e.g. HBV-N: ARHEIMER 1998; LIDÉN 2000). A fundamental prerequisite for water quality modelling at this scale is the adequate representation of hydrological processes (SINGH 1995). Irrespective of the ability of lumped models to capture daily runoff dynamics (e.g. JAKEMAN & HORNBERGER 1993), distributed models offer an advanced description of the variability of hydrologic variables and fluxes at different spatial scales. Distributed models are also essential to describe complex environmental scenarios and enable process-based, solute transport applications. Modelling of complex environmental systems always means a simplification of the natural system and therewith is subject to uncertainty. This is especially pronounced for the application of nutrient transport modelling and must be considered, when interpreting and dealing with model results.

Nordic landscapes are dominated by boreal forest and open land with distinct small scale landscape elements such as lakes and wetlands that have great influence on runoff generation and solute transport (e.g. BRANDESTEN 1987; GREN 1995). This mosaic of alternating landscape patches with individual characteristics needs to be addressed by the chosen model concept. Most conceptual hydrological models are to some degree spatially lumped and parameterised by effective parameters. These parameters are assumed to take into account spatial heterogeneity of landscape characteristics, meteorological variables and hydrological processes within a single model element. Depending on spatial discretisation effective parameters can neglect important hydrological processes and can be inappropriate in situations, where model discretisation exceeds small scale heterogeneity of relevant landscape characteristics. Typical measures to account for this so-called “sub-grid variability” are commonly used in macroscale applications (BLÖSCHL & SIVAPALAN 1995). They can consist of statistical distribution functions within a model element or a process adequate areal discretisations by subdividing model elements in different fractions (BECKER & BRAUN 1999). An essential element of distributed hydrologic modelling is the lateral routing of water along flow pathways (surface and subsurface) and stream flow for which different methods with varying complexity and data demand are available (e.g. SINGH 1995). Nordic environments are often characterised by stream networks intersected by various lakes and wetlands that often lack detailed geometric descriptions. Consequently only very simple lumped weighting functions are employed such as the triangular MAXBAS function of the HBV model (BERGSTRÖM 1992). If we want to use distributed models in such environments, there is a need for weighting functions that also account for spatial propagation of flow considering the retention effects of these lakes and wetlands.

Besides the consideration of distinct hydrologic characteristics of Nordic environments, the incorporation of nutrient transport under Nordic conditions was subject to several studies against the background of the implementation of efficient measures to reduce nutrient emissions (e.g. ARHEIMER 1998; ARHEIMER et al. 2004; DARRACQ et al. 2005). The complex processes involved regarding nitrogen turnover and transport processes for different land use regions, rivers, and lakes in combination with limited available input data, calls for robust conceptual routines with comparatively little data demand. A multitude of different approaches exists (e.g. ARHEIMER & OLSSON 2001). However, the application of a leaching coefficient methodology for distinct land use classes in combination with a simple empirical retention function coupled to a underlying hydrologic model is one of the most frequently found methodologies to account for nitrogen retention under Nordic conditions (e.g. HBV-N: ARHEIMER 1998; ARHEIMER & BRANDT 1998; LIDÉN 2000; ALEXANDER et al. 2000; DARRACQ et al. 2005). The applied models utilising this concept are mostly spatially lumped or operate on long term temporal scales. In view of this, fully distributed models offer the opportunity for spatially more realistic simulations of point and non-point source emissions and enable the spatial propagation and retention of nutrient loads along streams and lakes.

Successful conceptual model applications depend on accurate parameterisation. This is done by comparing observed and modelled stream flow at the basin outlet. This might be sufficient for simple lumped models, but is not a rigorous enough criterion for distributed model evaluation in order to ensure a correct representation of internal state variables (e.g. MROCZKOWSKI et al. 1997). Additional data such as groundwater levels or soil moisture measurements are required for a sufficient multi-criteria calibration procedure, but the availability of such data is limited or lacking in most real world applications.Multi-scale validation with runoff series from different catchments enables an advanced parameter estimation and may lead to a subsequent improvement of model consistency and performance (SOOROSHIAN & GUPTA 1995).

The most popular hydrological model in Scandinavia is the conceptual lumped HBV model (BERGSTRÖM 1976, 1992). It dates back to the early 70s and since then has been subject to continuous improvement and development. Besides the most recent HBV-96 release (LINDSTRÖM et al. 1997) and its nutrient transport derivate HBV-N (ARHEIMER 1998), numerous different HBV model versions are available, but only relatively few fully distributed and raster-based applications have been reported so far (e.g. BELDRING et al. 2003; SAELTHUN 1996). However, a number of raster-based models that are to some extent more conceptually or physically based have been developed (e.g. TAC^D: UHLENBROOK et al. 2004), but these models require detailed physiographic information for meaningful parameterisation.

1.1. Objectives

The objectives of this study were fourfold:

- Collection and procession of available spatial, hydrological, meteorological, and chemistry data in the Fyrisån catchment and its allocation in a central data base in order to provide consistent data for the model approach in this study and for further model applications. In addition, preparation and accomplishment of a two-day synoptic sampling campaign with the intention to gain additional snapshot information about the catchment-wide spatial nutrient pattern and the evolution of nutrients along the streams for additional model evaluation and testing.

- Introduction of a distributed, process-oriented catchment model based on the HBV model concept and demonstration of its applicability in a meso-scale low-land catchment with mixed land use. Furthermore the development of an efficient method to account for the sub-grid variability of land use parameters within a raster-based hydrological model and the integration of a simple routine for runoff routing in surface water bodies (channel network and lakes) in a low-land catchment.

- Implementation of nitrogen transport routines based on the concepts of HBV-N and TAC^D and calibration against observed water quality time series.

- Intensive model evaluation and testing of the hydrological model as well as the nitrogen transport model including the hierarchical scheme for systematic testing of hydrological simulations (KLEMES 1986), a comparison to the lumped HBV model version, and evaluation against obtained spatial patterns of stream flow and nitrogen concentrations.

1.2. Procedure

The procedure of this thesis was in general oriented on the specific order of the four main objectives stated in the prior section. Starting point for this thesis was the collection and procession of available input data of the Fyrisån catchment and its allocation in a central data base. Parallel to the input data procession, planning and preparation of the synoptic sampling campaign was done and synoptic sampling was carried out during the end of June 2005. The next step involved the data preparation and interpretation of the synoptic sampling campaign, which helped to identify potential problem areas and relations between land use and concentration patterns with regard to the later model application. After synoptic sampling the focus was directed to total nitrogen transport applications, as additional simulations of fractions of nitrogen or phosphorus were beyond the scope of this thesis with respect to the given time frame. The development and model evaluation in this study was carried out separately in order to allow an individual analysis and discussion of both models. The general approach is outlined in Figure 1.1 and was carried out in two steps:

The development and application of the hydrological model were the first objectives. The model was calibrated individually against observed runoff. Subsequent intensive model evaluation allowed to use the hydrological model as basis for the further implementation of the solute transport model.

Then, the solute transport model was developed and coupled to the already calibrated rainfall-runoff model that provides the hydrological driving variables. Thus, separate calibration of the solute transport model involved only solute transport model parameters that were optimised against observed nitrogen concentrations. A subsequent transport model application and evaluation followed.

The thesis finally concludes with the interpretation of the results of both model applications.

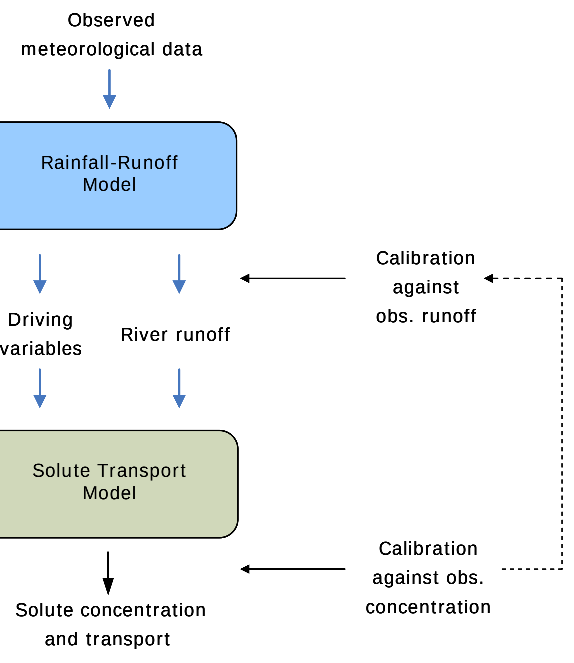

Figure 1.1: General approach for the model development and implementation of nitrogen transport routines (after LIDÉN 2000).

2. Background

Nitrogen plays a key role in many terrestrial, marine and freshwater ecosystems in controlling species composition, diversity, and functioning. Human activities have significantly altered the global nitrogen cycle (Vitousek et al. 1997). The rate of nitrogen input into the terrestrial cycle has approximately doubled mainly due to agricultural management practices and combustion of fossil fuels. As a consequence, the transfer of nitrogen through rivers has greatly increased. Numerous studies have been published on different aspects of nitrogen cycling and transformation processes at different scales. However, there is still a considerable lack of knowledge and ongoing debates about various aspects of the nitrogen cycle in the scientific community. This chapter intends to give a short overview of basic processes of nitrogen transformation, leaching, and transport in Nordic environments with regard to a further mesoscale nitrogen transport model application. More detailed descriptions and reviews of the current state of the research can be found in the literature (e.g. Allan 1995; Galloway et al. 2004; Haygarth & Jarvis 2002; Novotny 2003; Stevenson & Cole 1999; Stumm & Morgan 1996).

2.1. Nitrogen sources and transformation

2.1.1. Nitrogen leakage from the terrestrial system

Behaviour and transformation processes of nitrogen in soils, sediments of surface waters and lakes are complex and pathways from soil to surface waters are numerous and not well defined. Nitrogen occurs in soils and sediments in different chemical forms (e.g. as an ion, a dissolved gas or in solution with water) (Figure 2.1).

Dissolved inorganic nitrogen (DIN)
NO_3^- nitrate
NO_2^- nitrite
NH_4^+ ammonium
Dissolved organic nitrogen (DON)
Particulate organic nitrogen (PON)

Total dissolved nitrogen (TDN)

Total nitrogen

Figure 2.1: Major forms of nitrogen found in natural waters. Nitrogen is also present as N_2 gas (not shown) (after Allan 1995).

Tot-N in water is comprised of dissolved inorganic nitrogen, organic nitrogen and particulate organic nitrogen, minus N_2 gas. Phytoplankton and bacteria contribute to the amount of dissolved inorganic nitrogen content. Decomposition of aquatic life adds both dissolved organic and particulate organic nitrogen to water, while sewage runoff, erosion, and overland flow increase particulate inorganic nitrogen levels in water. Moreover bacterial denitrification converts nitrate to N_2 gas.

As a major plant-nutrient, nitrogen is often applied in large amounts to arable land in order to maintain optimal crop yields (e.g. Haygarth & Jarvis 2002). Further sources of soil nitrogen include atmospheric deposition, nitrogen fixation from the atmosphere by soil bacteria and legumes and plant residues. In addition to fertilising lawns, significant amounts of nitrogen enter soils from seepage areas of household septic systems in urban and suburban areas (NOVOTNY 2003). A schematic representation of the processes of nitrogen transformation is exemplified by the simple soil nitrogen cycle in Figure 2.2.

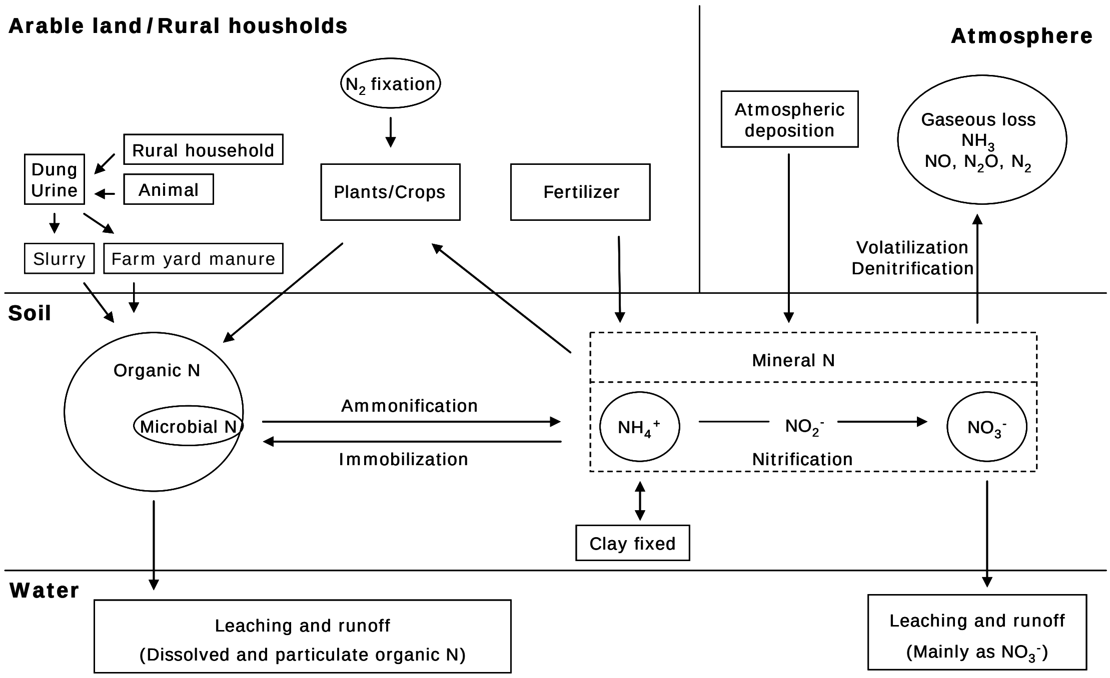

Figure 2.2: A simplified diagram of the soil nitrogen cycle (after HAYGARTH & JARVIS 2002).

Following major processes are part of the soil nitrogen cycle as defined by NOVOTNY (2003):

- *Nitrogen fixation* is a process by which soil micro organisms in symbiosis with leguminous plants utilise atmospheric nitrogen and change it to an organic form.
- *Nitrogen accumulation (bacterial uptake)* is the conversion of ammonium nitrogen to protein and cell tissue by heterophic soil organisms.
- *Ammonification* describes the process by which protein and other organic forms of nitrogen are decomposed to ammonium by biochemical breakdown of the proteins.
- *Decompostation (Hydrolysis of urea)* involves conversion to ammonium ions in the presence of the enzyme urease, which is provided by many heterotrophic organisms.
- *Nitrification* is a complex process occurring in soils and surface waters by which ammonium nitrogen (NH_4^+) is oxidised to nitrate (NO_3^-) with nitrate (NO_2^-) as intermediate product. Nitrification is thereby accomplished by two groups of chemotrophic bacteria, Nitrosomonas (oxidising ammonium to nitrite) and Nitrobacter (converting nitrite to nitrate).
- *Denitrification* is a process that occurs under anoxic conditions and usually occurs in water filled pores of soils. In aquatic sediments and substrates of wetlands, anoxic conditions always prevail, so surface sediment layer, only a few millimetres thick, can become aerobic. In wetlands, rhizomes of some plants have the capability of

transferring oxygen to their roots and creating aerobic pockets near the roots. During nitrification, NO_3^- serves as an electron acceptor and is reduced to gaseous reduced forms, including N_2, N_2O, NO and NO_2.

- *Fixation of ammonium* involves the sorption of NH_4^+ in between the layers of expanding clay minerals, such as monmorillonite. In this form, ammonium is considered unavailable for plant growth or bacterial uptake.
- *Ammonium volatilisation* occurs at high soil or water pH values when the ammonium ion (NH_4^+) is converted to gaseous ammonium (NH_3), which volatilises and is lost to the atmosphere.

Soil nitrogen is contained mainly in soil organic matter (>95 %) or in case of ammonium ions, it can be sorbed by clays and organic matter. In these form soil nitrogen is immobile and not available to plants. Nitrogen is lost from the soil primarily by erosion, crop harvesting, denitrification, NH_3 volatilisation, and nitrate leaching. Thereby the immobile forms can be converted to mobile forms that are available to plants and can be transported by soil water and infiltrate into groundwater. In general available mobile nitrogen constitutes only 0.1 % of the Tot-N in storage (e.g. STEVENSON & COLE 1999).

In this context, forms of reactive mobile nitrogen with known concern of water pollution, are NH_3, NO_2^- and NO_3^- (HAYGARTH & JARVIS 2002). Since ammonium is rapidly nitrified to NO_3^- by soil micro organisms and is held tightly to the negative charges of clay minerals and soil organic matter, it is relatively immobile and harmless. However, it can be subject to erosion and is then removed occasionally with overland flow. Nitrite, as intermediary product in the process of nitrification, has a short half-life and usually does not pose a problem. But under conditions of high temperatures and poor aeration NH_4^+ oxidation can exceed NO_2^- oxidation and lead to nitrite accumulation. In addition, high NO_3^- concentrations and high pH values can also cause NO_2^- accumulation and subsequent leaching. Nitrite is very reactive and toxic to aquatic life and under normal conditions only present in small quantities in soils and waters. The key process that mobilises nitrogen and promotes losses to water courses is the conversion of NH_4^+ to intermediate NO_2^- and further to NO_3^- by nitrifying bacteria. Nitrate is highly mobile, since it is relatively stable, very soluble and not fixed on clays or organic matter due to its negative chart. The problem of nitrogen leaching from soils to waters is mainly associated with NO_3^-, but also includes small amounts of NH_4^+ and NO_2^-. In addition, recent research revealed the importance of dissolved organic nitrogen leaching from soils, but still many aspects remain unknown (MURPHY et al. 2000).

There are two principal hydraulic pathways by which these mobile forms of nitrogen can be leached or transferred to waterways (HAYGARTH & JARVIS 2002). One is horizontal flow that occurs in soils with poor drainage on the soil surface or above impermeable layers within the soil. The other is vertical flow through the soil profile via matrix flow or through bypass flow in large macropores and cracks. Retention of mobile nitrogen in soils is therefore mainly dependent on soil properties, slope, position in the landscape and amount and frequency of rainfall events. Thus variability in terrestrial nitrogen leakage can be explained to a large extent by natural and human induced catchment characteristics, as well as by temporal hydro-meteorological conditions.

2.1.2. Nitrogen sources and retention in the aquatic system

The nitrogen load into surface waters normally originates from various point and non-point sources. Contributing point sources may be waste water treatment plants, industries and rural household emissions, while diffuse sources contain leakage from different land use forms, runoff from sealed surfaces, and atmospheric deposition on lakes and open water courses.

Nitrogen is subject to transformation during its transport in freshwater bodies. The long term discrepancy between the sum of all nitrogen emissions including leakage and the total catchment outflow is often referred to as retention (e.g. ANDERSSON et al. 2005; DILLON et al. 1991). Retention is hereby defined as a lumped expression for the net effect of various biogeochemical processes. The dominating processes responsible for temporary or permanent nitrogen removal from the water phase include mainly biological uptake, sedimentation and denitrification as shown in Figure 2.3.

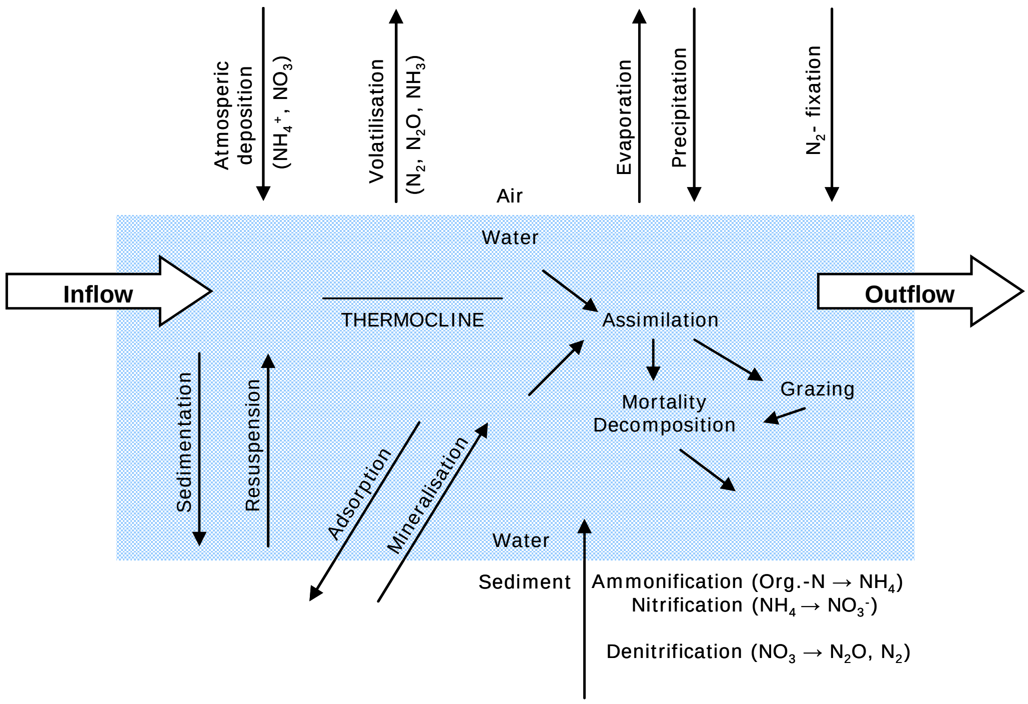

Figure 2.3: Major turnover processes affecting nitrogen concentration in a watershed (from ARHEIMER 1998).

From a modelling point of view, these processes may be related to hydrologic and climatic driving variables. Retention is closely linked to temperature, since an increase in temperature accelerates metabolic processes, such as denitrification and biological uptake, resulting in summer concentrations of nitrogen that are normally significantly lower in comparison to the rest of the year (e.g. SEITZINGER 1988). However, this decrease in inorganic nitrogen may be counteracted by nitrogen fixation and increased organic nitrogen concentrations by decomposition of phytoplankton in the water phase (e.g. JENSEN et al. 1992). Besides temperature another major factor influencing retention is residence time. Longer residence times allow more nitrogen removal from the water phase.

GREEN ET AL. (2004) found in a global analysis that on a basin wide scale an average nitrogen sequestration of 18 % was achieved through the combined effects of lakes, reservoirs, wetlands, and riverine systems based on residence time and temperature differences across the watershed.

Thus retention is favoured in situations where water is stored in the landscape. Groundwater, wetlands, streams, and rivers are key landscapes to environments and provide a continuum of environments with substantial capacity for denitrification, mainly due to abundant organic matter, sediments, and suspended particulate micro sites that offer anoxic environments. ARHEIMER (1998) characterised the influence of these distinct key landscape elements on nitrogen retention in more detail for Nordic environments:

- *Groundwater* denitrification occurs in recharge areas under the root zone and is favoured below the groundwater table were oxygen levels are low (e.g. FUSTEC et al. 1991). Moreover low nitrogen concentration levels have been observed in riparian zones. While some authors (e.g. CIRMO & MCDONNELL 1997) argue that relatively long residence times in combination with accumulation of organic matter and alterning saturation conditions favour groundwater denitrification in these zones, other authors suggested that these low concentrations might just be a result of different flow path and dilution of deeper groundwater (e.g. HILL 1990).
- *Wetlands* are considered as efficient nitrogen traps favoured by long residence times, alternating redox potentials, and anaerobic environments (e.g. CARPENTER et al. 1998; GREN 1995). Thus there has been great interest in constructing artificial wetlands for waste water treatment (e.g. GREN 1995) or for the reduction of diffuse source pollution (e.g. RAISIN & MITCHELL 1995). However, some authors (e.g. BERGSTRÖM 1991) questioned this effect for Nordic environments and argue that high hydraulic loads shorten the residence time and most transport occurs in late autumn or early spring, when biochemical activity is low.
- In *Streams*, sediments are the key environments for denitrification, as they provide the link between aerobic and anaerobic zones and have a high organic content (e.g. SEITZINGER 1988). Although the annual retention capacity of Nordic streams is only about 3 % of the total river load (e.g. SVENDSEN & KRONVANG 1993), denitrification can be quite effective on a seasonal basis or during river bank floods. Nevertheless in large low land streams, riverine retention was found to be more significant (e.g. SVENDSEN & KRONVANG 1993).
- *Lakes* are normally characterised by long residence times and by larger sediment surfaces in comparison to streams that favour denitrification. In addition sedimentation, water stratification and nitrogen fixation cause significant nitrogen reductions. While in shallow lakes sedimentation and thermal stratification play a minor role, these become more important in deeper lakes.

2.1.3. Link to catchment characteristics

As described in the prior sections the final concentration of nitrogen in stream water at the catchment outlet is the result of several processes involving terrestrial, aquatic, geological, and atmospheric interactions. According to VAGSTAD & DEELSTRA (2004) these processes can be summarised into:

- *Release and mobilisation* (e.g. mineralisation of organic nitrogen, sewage and industrial effluents).
- *Transport* (characterised by transit time and flow path e.g. leaching through the soil profile to groundwater systems, subsurface runoff).
- *Retention* (e.g. denitrification, sedimentation and adsorption along hydrological pathways).

These processes are spatially and temporally influenced and favoured by different conditions in the basin (e.g. land use, physiography, meteorology, hydrology and water management) (HAYCOCK et al. 1993). Thus the variability in stream flow can be assumed to be linked to the variability and heterogeneity in such characteristics (ARHEIMER 1998). This is the basic prerequisites for a spatially distributed and land use based dynamic model application in this study. Based on this assumption a model approach is pursued that incorporates distinct landscape characteristics. On the one hand it makes use of a leaching coefficient methodology depending on land use distribution. On the other hand it further relates retention to the identified key landscape elements regulated by residence time and temperature.

2.2. Models for nitrogen transport simulations

In general, modelling of nitrogen transport at the catchment-scale is very difficult. This is because of the complexity of the processes involved. A detailed description of an ecosystem encompassing all interacting components is not practical. Consequently, models make simplifications that suffer from uncertainties. In the case of nutrient transport modelling, uncertainty is increased by the fact that input data, such as diffuse or point sources that exert a direct influence on simulated loads, are normally affected with high uncertainty. Thus many approaches for modelling nutrient transport are based on empirical assumptions or employ spatial and temporal extrapolations (LIDÉN 2000).

Nevertheless, for watershed management it is essential to gain more knowledge about flow path and retention processes in order to enable an efficient environmental control and to introduce best management practices. Against this background, nitrogen transport models can be useful tools for analysing water quality issues. Based on simulations they can help to quantify contributions from various sources and to distinguish between natural variability and anthropogenic impact. Furthermore, modelling enables predictions of the future by scenario simulations. Models are often used for predicting the consequences of alternative management scenarios, planning, and policy level activities and can help to reduce costs of managing water resources and water quality in catchments.

In recent years numerous different approaches of estimating riverine loads of nitrogen, retention in streams, and terrestrial leakage have been developed. In general, nitrogen transport models can be divided into steady-state and dynamic models (ARHEIMER 1998):

Steady-state models have no time component and describe average temporal conditions for the application period. They may be based on hydrological model outputs, but mostly employ export coefficient methods or statistical and regression techniques. While the latter are also common for spatial and temporal extrapolation and source apportionment (e.g. GRIMVALL & STALNACKE 1996), export coefficient models utilise small scale measures and relate these to larger catchment areas (e.g. JOHNES 1996). According to ARHEIMER (1998), steady-state models can be further categorised according to the spatial starts for the calculation into:

- *Imission models*, i.e. models that relate estimated nitrogen transport or concentrations at the catchment outlet to upstream characteristics (e.g. BAUDER et al. 1993; GRIMVALL & STALNACKE 1996).
- *Emission models*, i.e. models that describe the conditions at the outlet of the catchment based on leakage coefficients and emission data within the catchment (e.g. HAITH & SHOEMAKER 1987; JOHNES 1996).

Dynamic models include time dependent process descriptions. These types of models are normally more data demanding and applicable only to catchments with available information about point and diffuse sources as well as information about transport processes involved. Advances in rainfall-runoff modelling enabled the development of process-based nutrient transport models. Such models are often coupled to hydrologic models, since riverine nitrogen load and concentration variability is closely linked to hydrological variability. As process-based models, they attempt to simulate transport processes by the describing the governing physical and biochemical processes. Dynamic process-based models may be further categorised by the level of distribution in time and space or by the degree of process description:

- *Physically based models,* i.e. models that are based on physical, chemical and biological laws with no empiricism involved. They aim at a full description of all processes involved and coefficients are derived from field experiences. By definition physical models must be distributed to account for the heterogeneity of the systems they are applied to.
- *Conceptual models*, i.e. models that only account for the dominating processes with parameter and coefficients that are derived empirically or by calibration.

Today a large number of models exists that enable water quality modelling at the catchment-scale. Table 2.1 intends to give an incomplete overview about models commonly used for water quality applications in Europe. Although a large variety of model concepts exist not many model intercomparisons can be found in the literature (e.g. ARHEIMER & OLSSON 2001).

Table 2.1: Common water quality models for the catchment-scale with applications in Europe (from ARHEIMER & OLSSON 2001).

Model name	Purpose	Process description	Reference
AGNPS	nutrients, pesticides	conceptual	YOUNG et al. (1989)
HBV-N	eutrophication control/ nitrogen transport	conceptual	ARHEIMER (1998)
INCA	eutrophication control/ nitrogen transport	conceptual/mechanistic	WADE et al. (2004)
MAGIC	acidification control/ nitrogen transport	conceptual/mechanistic	COSBY et al. (1995)
MIKE SHE	eutrophication control/ nitrogen transport / pollutant transport	mechanistic	REFSGAARD et al. (1999)
SWAT	eutrophication and pesticide control /sediment, nutrients, pesticides	conceptual	ARNOLD et al. (1998)

Since the first idea of a physically-based model by FREEZE & HARLAN (1969) and a plethora of diverse process-based physical or conceptual model concepts later, the classic question of adequate model complexity and predictive power has been debated in the hydrologic community (e.g. BEVEN 1989, 1993; BEVEN 1996; CHRISTOPHERSEN et al. 1993; GRAYSON et al. 1992; JAKEMAN & HORNBERGER 1993; REFSGAARD et al. 1996; SEIBERT 1999a). While physical-based distributed models are considered by some authors as the only possible way of simulating processes such as water quality (e.g. REFSGAARD et al. 1996), others question their limited applicability mainly due to massive input data constrains and the problem in up-scaling of plot scale derived experimental results and equations to the model scale (e.g. BEVEN 1996; GRAYSON et al. 1992).

In contrast to physically based models, the major advantage of conceptual models lies in their demand for less input data and makes them suitable for large-scale studies, and catchments with limited input data. However, models face problems of equifinality. This has been defined by BEVEN (1993) as the phenomenon that equally good model simulations might be achieved with many different parameter combinations. Equifinality causes uncertainty when using a model outside the calibration range and with different variables. It may indicate that the model is ill-posed (e.g. KUCZERA 1997), i.e. too complex for the rainfall runoff data used in calibration. The limited information inherent in rainfall runoff data calls for a parsimonious model and illustrates the basic dilemma formulated by KUCZERA & MROCZKOWSKI (1998):

"A simple model cannot be relied upon to make meaningful extrapolative predictions, whereas a complex model may have the potential but because of information constrains may be unable to realise it."

This dilemma is prominent for nitrogen transport modelling that requires a detailed and distributed description of processes and defines the challenge to find an appropriate middle course between parsimonious and complex alternatives in model development. The subsequent model development and application in this study was guided by a statement of BERGSTRÖM (1998) about prior attempts to incorporate water quality into the HBV model:

"The conclusion is that it can be made, if the level of ambition is realistic"

3. The Fyrisån catchment

The study took place in the mesoscale Fyrisån catchment (Figure 3.1) which is situated in the eastern part of the Central Swedish Lowlands 60 km north of Stockholm. It belongs to the Mälaren-Norrström drainage basin and covers an area of approximately 2000 km² before it discharges into Lake Ekoln, a northern branch of the lake Mälaren system which drains further into the Baltic Sea. The drainage area is crossed by the 60th parallel and extends between latitudes 59°37’ and 60°20’N and longitudes 17°04’ and 18°15’E. Several previous investigations were carried out in this research area before including the fundamental work of HJULSTRÖM (1935) on the morphological activity of rivers. More recent studies dealt with fluvial sediment transportation (e.g. GRETENER 1994), nutrient transport modelling (e.g. KVARNÄS 1996; DARRACQ et al. 2005), and the application of various hydrologic catchment models (e.g. SEIBERT 1997, 1999b; MOTOVILOV et al. 1999; XU 1999).

3.1. Morphology, topography and land use

The landscape is topographically and morphologically characterised by the very low-lying and flat Precambrian peneplain with most parts of the area ranging between 30 and 50 m above sea level and a highest point of 110 m. The area of elevated plateaus and hills is mostly covered by forests (60 %) of pine and spruce or a smaller fraction of mixed deciduous woodland, whereas the river valleys in the south particularly around the city of Uppsala are gradually substituted by agricultural fields (32 %). Wetlands with varying extents are numerous (4 %) and spread over the lower reaches of the catchments. Lakes constitute 2 % of the landscape and the majority is small with a mean surface area of 0.4 km² (GRETENER 1994). The two largest lakes are Vendelsjön and Dannemorasjön in the northern part of the catchment with areas of 4.2 and 4.0 km². The overall lake size ranges from 0.01 to 4.2 km² with mean depth varying from 0.8 to 6.4 m. Besides the city of Uppsala, settlements (2 %) are generally small in extent and scattered over the area and only a small portion can be regarded as sealed.

The distribution of predominant soil types can be roughly related to land use information. Clay soils constitute most parts of the farmland in the region, while till soils are generally covered by forest (SEIBERT 1999b). Till is the most common soil type in the research area and dominates in the north. The thickness of till is variable and greater depth of 10 to 20 m can be found in the western part, while fine-grained clay soils in combination with sandy and silty material dominate in the south, where glacial clays can reach depth of up to 15 m.

The geology in the research area is part of the Baltic shield that is characterised by a mosaic of granitic and metamorphic rocks. The bedrock geology is dominated by granites, but also supracrustal rocks such as leptide, gneiss, and hälleflinta occur frequently. Leptide in the northwestern part of the catchment around Dannemora contains iron and was subject to intensive mining in Swedish history (SEIBERT 1994).

Today’s appearance of the landscape in the Fyrisån was strongly influenced by quaternary glaciation and consists largely of glacial deposits with eskers and outcrops of bedrocks rising over the plain. Ice recession from the Fyrisån basin was directed largely from south to north. Lower recession rates are evident by series of moraines and the region is crossed by N-S oriented eskers that can reach a height of 20 to 50 m. One example is the Uppsala-esker that runs through Uppsala and extends northerly until Billuden. The Uppsala-esker provides important groundwater resources for the city of Uppsala (SEIBERT 1994).

The small relief makes it generally difficult to define catchment divides in the region. The Fyrisån is classified as a low gradient river and consists of five main tributaries, the Rivers Vendelån, Vattholmaån, Björklingeån, Jumkilsån, and Sävjaån. It is interesting to note that in the literature different source areas are mentioned. While GRETENER (1994) refers to the River Vendelån as the source area of the Fyrisån, in other publications (e.g. KVARNÄS 1996; LARSSON et al. 1998) the River Vattholmaån is regularly labelled as Fyrisån. The latter notion was also adopted for this study (Figure 3.1).

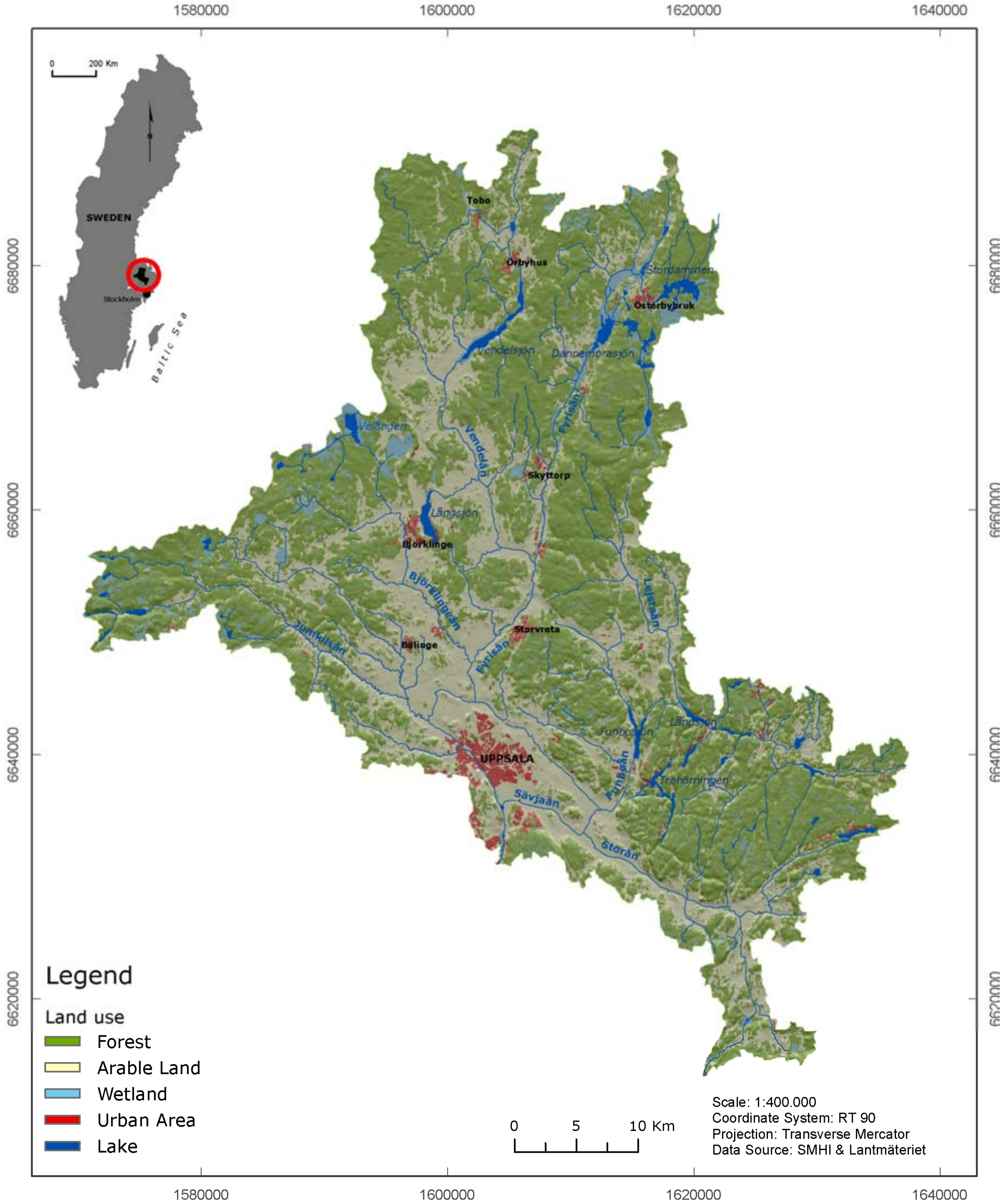

Figure 3.1: Overview of the Fyrisån catchment.

Drainage of the Fyrisån is oriented in a north-south direction following mainly the same drainage direction of the last Weichselian glaciation. However, on a local scale the tributaries and the main branch of the Fyrisån follow valleys along fault lines and fissures, forming a rectangular-to-parallel drainage pattern (GRETENER 1994). In Figure 3.1 this pattern is visible for the tributaries Björklingeån and Jumkilsån flowing towards the east on almost parallel courses and for the River Sävjaån running towards the northwest in a fissure valley that is the continuation of the River Jumkilsån valley.

3.2. Climate

The research area is located within a region of relatively low annual precipitation with a corrected mean annual precipitation for the meteorological station Uppsala of 543.6 mm a^{-1} for the period 1855 to 1970 and an increase towards the west as well as the east somewhat above 700 mm a^{-1}. Maximum precipitation is observed in August and minimum in February and March being typical for continental type climate conditions (SEIBERT 1994) (Figure 3.2). Low monthly amounts of precipitation are usually in winter. Frontal depressions are the major weather pattern. In the Fyrisån, approximately 50 % of the rains are frontal-oreigenic and about 50 % are convective. In the summer local rainfall is usually caused by convectional activity and often yields high intensity rainfalls combined with frontal zones. Snow constitutes about 20-30 % to the total precipitation with an average duration of snow cover of 100 to 110 days per year. The mean date of first day with a snow cover is in the middle of November. Thickness of the snow cover varies from year to year and reaches its maximum usually in February, with average maximum depth ranging from 30-50 cm. The mean annual temperature of the period 1855 to 1979 for the station Uppsala is +5.2 °C. February is statistically the coldest month with normal means of -5 °C, whereas July is the warmest month with normal means of +17 °C. The vegetation period lasts 180 days.

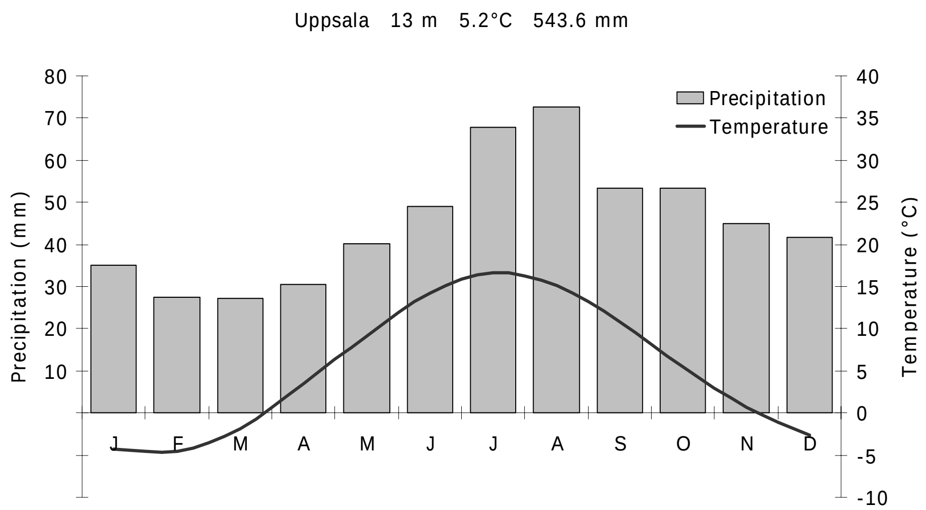

Figure 3.2: Climate chart for the city Uppsala for the period 1855 to 1970.

3.3. Hydrology

The runoff regime shows a typical Baltic regime with a dominant primary snowmelt spring flood in April and a secondary rainfall peak flow in autumn intermitted by a low flow period during the summer month (GOTTSCHALK et al. 1979). Groundwater storages are usually filled in early spring so that excess water from snow melt or precipitation is likely to cause quick runoff responses and increasing discharges. During summer the potential evaporation increases and the water reserves are gradually depleted, even though precipitation may be relatively high, resulting in usually lower summer and autumn discharges (GRETENER 1994). In autumn precipitation normally suffice to refill the water storages and shows a second peak in discharge. This pattern reflects long term average behaviour of the system. However, on short term-basis irregularities exists and unstable regimes can occur, since the hydrological behaviour is closely linked to the influence of climatic factors as well as human influence. The climatological conditions of the Fyrisån drainage basin are largely responsible for the general hydrological response and can be summarised in the water balance table for the main runoff stations in the region (Table 3.2). Characteristic runoff values are given in Table 3.1 for the period 1981 to 1991. Typical values for high runoff in the Fyrisån catchment range from 40 to 70 l s^{-1} km^2 (SEIBERT 1994).

Table 3.1: Characteristic values of runoff of main discharge stations in the Fyrisån catchment for the period 1981 to 1991 (from SEIBERT 1994).

Name of station	HHq (l s^{-1} km^{-2})	MHq (l s^{-1} km^{2})	LHq (l s^{-1} km^{-2})	HMq (l s^{-1} km^{2})	MMq (l s^{-1} km^{2})	LMq (l s^{-1} km^{2})	HLq (l s^{-1} km^{-2})	MLq (l s^{-1} km^{2})	LLq (l s^{-1} km^{-2})
Vattholma N. Bro	50.70	29.83	15.85	14.20	8.55	5.40	2.43	1.08	0.32
Date	*09.04.82*		*22.03.91*				*13.08.81*		*03.08.89*
Sävjaån	72.90	39.19	19.53	10.62	7.69	4.23	1.51	0.64	0.14
Date	*23.04.85*		*17.01.89*				*25.07.87*		*12.09.89*
Ulva Kvarndamm	46.32	31.91	19.16	12.03	7.03	4.58	1.47	0.87	0.38
Date	*08.04.82*		*16.01.89*				*25.07.87*		*12.09.89*

Table 3.2: Water balance of main discharge stations in the Fyrisån catchment for the period 1981 to 1991 (from SEIBERT 1994).

Name of station	Precipitation (mm a^{-1})	Evaporation (mm a^{-1})	Runoff (mm a^{-1})
Vattholma N. Bro	750	482	268
Sävjaån	732	488	245
Ulva Kvarndamm	755	534	222

3.4. Chemistry

In general nitrogen concentrations found in surface waters in the Fyrisån catchment are high due to intensive land use in combination with various point sources (sewage treatment plants and rural household emissions). Continuous records at the station Flottsund that describes the water chemistry at the catchment outlet, exhibit since 1965 the high annual concentration values of the Swedish Environmental Quality Criteria (e.g. LARSSON et al. 2000). Figure 3.3 illustrates the constant high nitrogen concentrations since 1990, while Figure 3.4 states the spatial evolution along the Fyrisån for the last five years per station. At Flottsund a decrease in total nitrogen concentration could be observed in recent years, what might be a result of improved nitrogen treatment since the year 2000 by the Uppsala water treatment plant (e.g. LARSSON et al. 2000). In Figure 3.4 forested areas show smaller concentration ranges for the last years, while stations characterised by higher arable land percentages show consistent higher values.

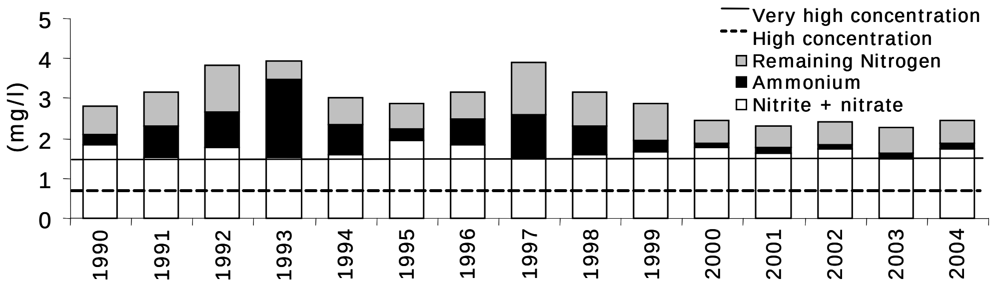

Figure 3.3: Tot-N concentrations observed at the outlet of the Fyrisån catchment for the period 1995 to 2004.

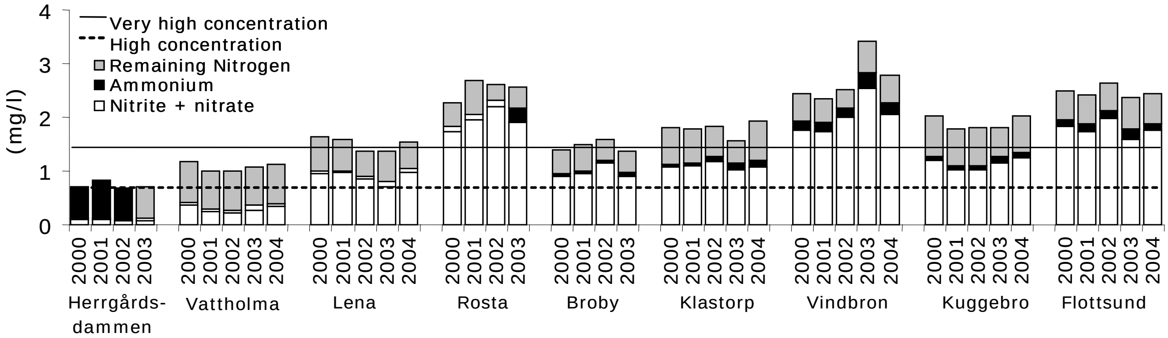

Figure 3.4: Evolution of Tot-N concentration values along the Fyrisån for the period 2000 to 2004.

4. Model development

4.1. Software framework

4.1.1. PCRaster

PCRaster is a dynamic modelling system for distributed models including raster GIS functionality. It provides a modern environmental modelling language (EML) for constructing models which describe processes through time based on a rich set of predefined functions or externally developed and compiled functions. The concept of PCRaster realises a high-level linkage between the dynamic section of a modelling system and the GIS, with a direct link to an underlying spatial GIS data base. That is why PCRaster is also referred to as a dynamic GIS (VAN DEURSEN 1995).

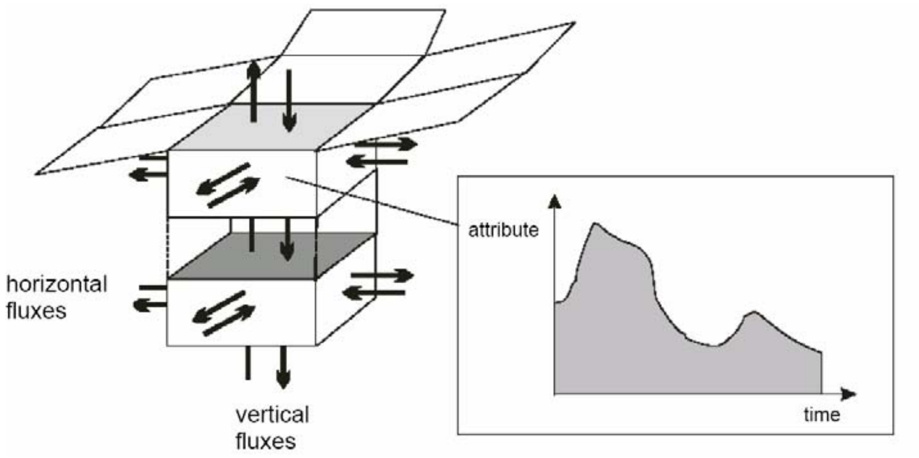

Figure 4.1: Spatial fluxes and time variable cell attributes (after VAN DEURSEN 1995).

Figure 4.1 exemplifies the spatio-temporal concepts of the PCRaster environment. A system that is subject to a modelling approach with PCRaster is discretised in grid cells and different attributes can be assigned. Lateral and vertical information can be exchanged by different neighbourhood operations and since a vertical layered map stack can simulate a 3 dimensional structure, this approach is also called 2.5 dimensional. Input and output of PCRaster based simulations are raster maps and time series. In general PCRaster provides a modelling environment that is specially designed for hydrologic modelling purposes and simplifies the application of different model concepts.

4.1.2. PEST

In this study an automated model calibration procedure was applied by coupling the model to the parameter estimation programme PEST (Parameter ESTimation). PEST is a model-independent, nonlinear parameter estimation and optimisation package, frequently used for model calibration in different research fields (DOHERTY 2005; DOHERTY & JOHNSTON 2003). It is based on the implementation of a Gauss-Marquardt-Levenberg algorithm which combines the advantages of the inverse Hessian method and the steepest descent method to allow a fast and efficient convergence towards the objective function minimum. The best model parameter set is selected within a specified range of parameter values by minimising the discrepancies between model results and simulated or predefined values in a weighted least square sense.

Coupling with PEST is achieved by linking PEST to the respective in and output files of the hydrologic or nutrient transport model. This enables PEST to read model outputs and relate them to predefined or measured values and to write parameter input files for the next model run. Optimisation is achieved in an iterative procedure of running the model with a specific parameter set selected by PEST, reading the model output files after the model ceased execution and choosing a new parameter set based on the Gauss-Maquardt-Levenberg algorithm. Several parameters and options exist to influence the optimisation process and to achieve a better optimisation result.

A PEST derivate, called Parallel PEST, was applied in this study due to the high computational requirements of the developed model. In contrast to PEST that is limited to a single personal computer Parallel PEST allows the parallelisation of the optimisation process by the simultaneous use of several personal computers. While PEST resides on a single machine, model runs are carried out simultaneously on different network machines and communication and access to model in and output files is assured over the computer network. Clients can be connected, started or stopped anytime, as PEST redistributes dynamically the required model runs between different machines. To achieve realistic computation times and efforts in the actual study, up to six machines with a maximum of ten instances of parallel model runs were involved in the optimisation process.

4.2. Hydrological model

4.2.1. Basic model concept

The model concept applied in this study is a refined and fully distributed (grid based) version of the conceptual rainfall runoff model HBV (BERGSTRÖM 1992) with a spatial resolution of 250 × 250 m². This distributed HBV model simulates daily discharge by using daily precipitation and temperature as well as monthly evapotranspiration estimates as input. It shares with the original HBV model the same sequentially linked routines and functions representing all processes of the land phase hydrological cycle. The model structure starts with a snow module, simulating snowmelt with the degree-day method, is followed by a soil routine, where groundwater recharge and actual evaporation are functions of actual water storage in a soil box and ends with a runoff generation routine where runoff formation is represented by linear storage equations. Detailed descriptions including the governing equations can be found in BERGSTRÖM (1976; 1992).

Key elements for the spatial distribution of the model were adopted from the distributed and process-oriented catchment model TAC^D (tracer aided catchment model, distributed) (UHLENBROOK et al. 2004; UHLENBROOK & SIEBER 2005). These core elements contain the modular structure with a specifically designed runoff generation routine and the integration in the geographical information system PC-Raster (KARSSENBERG et al. 2001). PC Raster offers a dynamic modelling language for raster based applications and enables lateral cell to cell routing with the single-flow direction algorithm (D8) (O'CALLAGHAN & MARK 1984).

The distributed HBV model was optimised to the prevailing topographic and morphologic features of the lowland Fyrisån catchment. Runoff generation was parameterised separately according to predominating distinct landscape elements (forest, arable land, urban areas and wetlands) and applied along with a sub-grid parameterisation scheme. A simple lake and flow distribution routine was developed to account for low land streams interconnected by lakes. In this manner, the model enables dynamic simulations of water flow in all stages of the hydrological cycle that can be subject to calibration and validation against temporal and spatial observations. Figure 4.2 illustrates the structure of the hydrologic model in this study. The different modules are discussed in the next chapters following the sequential order of the model structure.

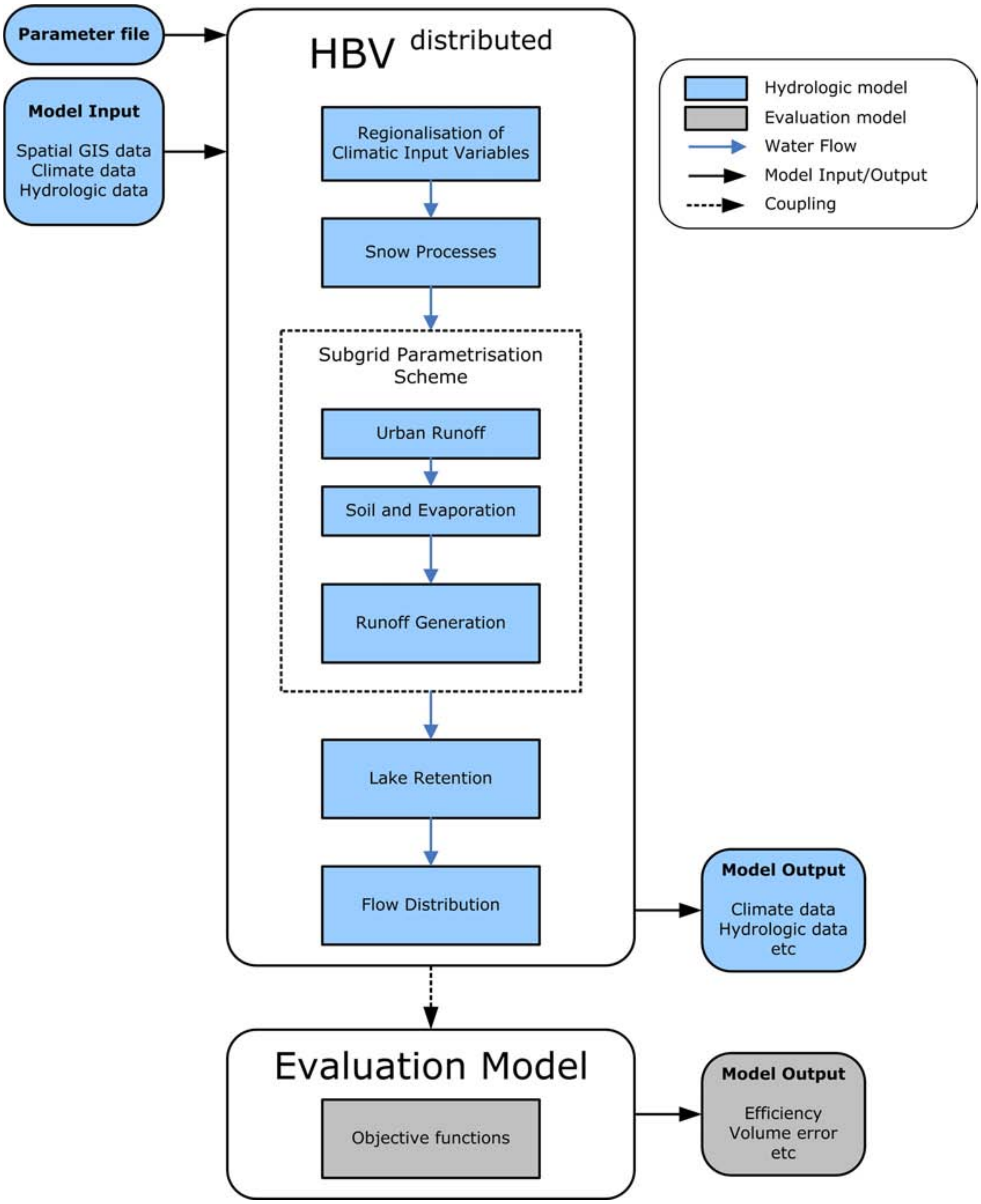

Figure 4.2: Schematic structure of the hydrological model.

4.2.2. Regionalisation of climatic input variables

An accurate description of input variables is most essential for successful and accurate rainfall runoff modelling. The choice of regionalisation and correction methods to transform point measurements into spatial data depends on several factors, such as the number and location of measurements as well as climatological and topographical considerations.

To correct precipitation according to elevation an increase of about 10 % in precipitation per 100 meters is assumed in Sweden, while for temperature the lapse rate is normally set to the wet adiabatic rate of -0.6 °C per 100 m increase in elevation (BERGSTRÖM 1976, 1992). In the case of the Fyrisån drainage basin no elevation lapse rates had to be considered, since prevailing elevation differences were mainly within 30 m. The HBV model is relatively robust with regard to systematic errors within areal climatological data, since it is inherently accounted for by the model parameters during calibration (e.g. LIDÉN 2000). The highest bias occurs during snowfall. A snowfall correction factor (*SFCF*) is introduced within the snow routine integrating several effects such as systematic measurement errors and evaporation from snow (cf. 4.2.3).

Regionalisation of input data was done for precipitation and temperature records employing an inverse distance weighting method. This method weights the influence of each station in respect to its distance based on following expression:

$$z(x_0) = \frac{\sum z(x_i) \cdot d_i^{-r}}{\sum d_i^{-r}} \qquad \textbf{Eq. 4.1}$$

$z(x_0)$: Interpolated value at location x_0
$z(x_i)$: Measured value at gauging station x_i
d_i: Distance to gauging station (m)
r: Weighting coefficient of reciprocal distance

Potential Evapotranspiration for the HBV model is usually provided as monthly mean estimate (ERIKSSON 1981) based on the Penman formula (PENMAN 1948) and was considered as sufficient within this model application. LINDSTRÖM ET AL. (1997) compared a number of alternative calculations of evapotranspiration for the HBV-96 model, but found that none of these gave significantly better results for runoff simulations.

4.2.3. Snow accumulation and melt

The snow routine was adopted from the HBV model and employs a simple degree-day relation based on air temperature and a water holding capacity of snow to delay runoff. Snow routine inputs are daily precipitation and temperature data, while effective precipitation (liquid precipitation and melt water) constitutes the output to the underlying soil routine. The snow routine is parameterised by five parameters (*SFCF*, *TT*, *CWH*, *CFR* and *CFMAX*).

The type of precipitation is controlled by a temperature threshold parameter *(TT).* It is regarded as a free parameter that depends on the topographical characteristics of a catchment, but also accounts for inaccuracies of areal air temperature (e.g. KIRNBAUER et al. 1994). In order to capture the delayed melting in forests in comparison to open land in the model simulation, *TT* is treated separately for these land use classes and is normally close to 0 °C. If air temperature drops below *TT*, precipitation is assumed to be in the form of snow. In this case a snowfall correction factor (*SFCF*) is applied to account for wind-induced errors from point precipitation measurements. While no description of evaporation losses from snow is included within the model concept, it is implicitly dealt with by the *SFCF* parameter. Like the parameter *TT*, *SFCF* is adjusted independently for forest and open land. This distinction is based on results from SEIBERT (1999b), who showed that *CFMAX* decreases if the forest percentages in catchments are increasing. In this case the snowfall correction factor compensates for the fact that evaporation of snow in forested areas (e.g. LUNDBERG & HALLDIN 1994) is not explicitly captured by the model, since lower values of *SFCF* reduce the water equivalent of the snow pack.

In the following section the governing equations of the snow module are presented starting with the aforementioned correction of solid precipitation:

$$Corrected\ precip = Observed\ precip \cdot SFCF \qquad if\ T < TT \tag{Eq. 4.2}$$

Corrected precip:	Corrected solid precipitation (mm d^{-1})
Observed precip:	Observed precipitation (mm d^{-1})
SFCF:	Snowfall correction factor (-)

TT defines the temperature above which snow melt occurs. Snowmelt is calculated subsequently according to the degree day equation:

$$Snowmelt = CFMAX \cdot (T\text{-}TT) \tag{Eq. 4.3}$$

Snowmelt:	Melt water of snow (mm d^{-1})
CFMAX:	Degree-day factor (mm °C d^{-1})
T:	Mean daily air temperature (°C d^{-1})
TT:	Threshold temperature (°C d^{-1})

As long as the amount of melt water does not exceed a certain fraction, defined by the retention capacity parameter *CWH*, the snow pack can retain melt water. *CWH* is normally confined to a value of 0.1 for applications in Sweden (BERGSTRÖM 1976):

$$Water\ content = CWH \cdot Snowpack \tag{Eq. 4.4}$$

Water content:	Water content of snow cover (mm d^{-1})
CWH:	Coefficient of water retention capacity (-)
Snowpack:	Water equivalent of snowpack (mm d^{-1})

This water refreezes again when temperature decreases below *TT*. Hence the correction factor *CFR* is applied to the degree day equation. In Sweden a value of 0.05 is commonly used for the parameter *CFR* (BERGSTRÖM 1976).

Refreezing melt water = CFR · CFMAX · (TT-T) **Eq. 4.5**

Refreezing melt water:	Amount of melt water that refreezes (mm d^{-1})
CFR:	Refreezing coefficient (-)

This simple conceptualisation of fundamental processes of snow accumulation and melt was subject to intensive discussion and improvement attempts (e.g. LIDÉN 2000; LINDSTRÖM et al. 1997). For instance LIDÉN (2000) noted that the exclusion of important variables such as wind speed, albedo of the snow, solar radiation, snow evaporation and soil temperature seems unjustifiable. Nevertheless, LINDSTRÖM ET. AL (1997) showed that the introduction of more advanced routines and additional input data had only limited effects on the result of snow modelling. This is also in line with findings of a WMO intercomparison of snowmelt models confirming that advanced snow modelling routines do not necessarily result in better runoff simulations (WMO 1986).

4.2.4. Urban runoff

The urban runoff routine accounts for urban areas with a high proportion of sealed surfaces, such as paved roads, densely populated areas or rocky outcrops that are assumed to be connected to a central sewage water system or to directly drain into streams and thus constitute to quick runoff response in the river channel. The routine implements a split parameter (*UrbanSplit*) that determines the fraction of precipitation of the urban runoff generation type directly entering the next stream, while the remaining fraction can further infiltrate into the soil. Lateral routing of urban runoff into streams is performed instantaneously within the same model time step. The implementation of the urban runoff routine was considered adequate, as the city of Uppsala (>120000 inhabitants) constitutes most of the 34 km² of urban area, while remaining settlements show a more rural character.

4.2.5. Soil moisture accounting

The soil moisture accounting routine originates from the HBV model and is a key element of the model controlling runoff formation. It is based on three parameters *BETA*, *LP* and *FC*. *FC* determines the maximum storage capacity of the soil moisture storage and interception storage. *BETA* accounts for different infiltration characteristics of soil and *LP* is the soil moisture value above which evaporation reaches its potential value.

The calculation of soil moisture dynamics, infiltration and percolation is based on following assumption: The discharge of excess water from the soil (*ToRunoffGeneration*) is related to infiltration from rain or melt obtained from the snow module (*InSoil*) and depends on a ratio between actual soil moisture (*SoilMoisture*) and field capacity (*FC*) in combination with the empirical parameter *BETA* (Figure 4.3):

$$\frac{ToRunoffGeneration}{InSoil} = \left(\frac{SoilMoisture}{FC}\right)^{BETA}$$ **Eq. 4.6**

ToRunoffGeneration:	Infiltration into the runoff generation routine as a fraction of the actual soil moisture (mm d^{-1})
InSoil:	Input into soil routine (mm d^{-1})
SoilMoisture:	Actual soil moisture (mm)
FC:	Maximum of soil moisture storage (mm)
BETA:	Empirical parameter (-)

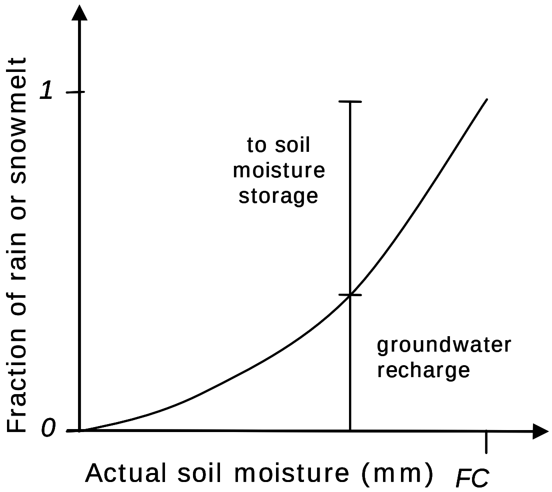

Figure 4.3: Contribution from rainfall or snowmelt to the soil moisture storage and to the upper groundwater zone (after SEIBERT 2002).

This simple conceptualisation of soil showed to be very robust and therefore has been frequently adopted in other models (e.g. ARNO: TODINI 1996). One advantage is the variability of the approach to describe both the physical properties of the soil and their statistical distribution per grid cell with comparatively little parameterisation effort. In the current study *FC* and *BETA* were parameterised individually according to the predominating land use classes (forest, agriculture, wetland and urban). This proceeding was based on the assumption that land use can be used as an indicator for underlying soil characteristics in the research area (cf. 3).

Actual Evapotranspiration within the soil routine is derived from a function of potential evapotranspiration and available soil moisture depending on the parameter *LP*. Starting from field capacity (*FC*) down to a limit of minimum soil moisture given by *LP*, actual evapotranspiration equals potential evapotranspiration. Below this limit a linear reduction is assumed (Figure 4.4):

$$ActET = PotET \qquad \text{if } SoilMoisture \geq LP \cdot FC \qquad \textbf{Eq. 4.7}$$

$$ActET = PotET \cdot \frac{SoilMoisture}{LP \cdot FC} \qquad \text{if } SoilMoisture < LP \cdot FC \qquad \textbf{Eq. 4.8}$$

ActET:	Actual evaporation (mm d^{-1})
PotET:	Potential evaporation (mm d^{-1})
SoilMoisture:	Soil moisture (mm)
LP:	Reduction parameter of field capacity (-)
FC:	Field capacity (mm d^{-1})

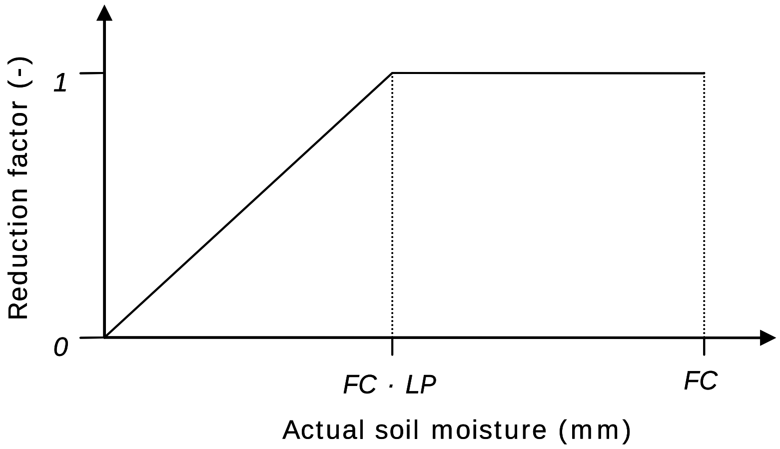

Figure 4.4: Reduction of potential evapotranspiration (from SEIBERT 2002).

Actual evaporation is subtracted subsequently from the soil moisture storage and evaporation is not assumed to occur in case of a snow cover. The parameter *LP* is parameterised depending on land use class analogue to the soil parameters.

Interception is addressed implicitly by evapotranspiration losses from the soil routine and by the snowfall correction factor. The incorporation of interception storages was tested by LINDSTRÖM ET AL. (1997) for the HBV-96 model and resulted in no significant improvements for runoff simulations in Sweden.

4.2.6. Runoff generation

Basic concept

The runoff generation routine is a response function transforming excess water from the soil routine to runoff. It is based on the linear reservoir concept, where runoff *Q(t)* at time *t* is supposed to be proportional to the water storage *V* and can be expressed by following fundamental differential equation (Figure 4.5):

$$-\frac{dV}{dt} = k \cdot V(t) = Q(t) \qquad \textbf{Eq. 4.9}$$

V: Storage level (mm)
t: Time step (time step)
k: Storage coefficient (1 time step^{-1})
Q: Flux (mm time step^{-1})

The solution for an instantaneous Dirac impulse at time $t = 0$ is given by following exponential equation and describes the outflow recession of a linear reservoir (Figure 4.5):

$$V(t) = V_0 \cdot e^{-kt} \qquad \textbf{Eq. 4.10}$$

V(t): Storage level at time t (mm time step^{-1})
V_0: Storage level at time t = 0 (mm time step^{-1})

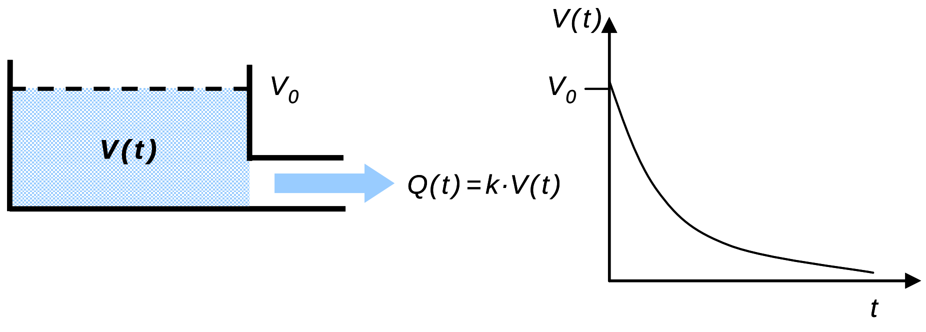

Figure 4.5: Linear storage and its outflow recession to an instantaneous Dirac impulse (after SEIBERT 2002).

Based on this fundamental principal, runoff generation processes are conceptualised separately for each land use class by applying individually adapted and parameterised linear storage concepts. These can consist of one simple linear reservoir or a sequential order of vertical connected linear reservoirs representing different runoff components, such as shallow and deep groundwater storages. The actual water content of linear storage depends on several aspects: initial water content, percolation from soil, lateral and vertical inflow and connection of storages in combination with individual outflow characteristics determined by parameterisation.

Based on the sub-grid parameterisation scheme (cf. 4.2.7), grid cells can contain certain fractions of different land use classes. However, lateral interconnection of storages is only enabled on a grid cell level. It is based on a local drain direction network (LDD) utilising the single-flow direction algorithm (D8) (O'CALLAGHAN & MARK 1984) and was derived from a digital elevation model (DEM). This algorithm ensures that each grid cell drains into one of its eight surrounding cells following the steepest topographical gradient. If grid cells contain a topographic depression a pit cell is assumed and lateral routing ends at this specific grid cell. In case of a sound LDD, this grid cell determines the catchment outlet.

Conceptualisation of runoff generation

The core element of the hydrologic model is the runoff generation routine, since it controls the dynamics of generated runoff and allows the incorporation of dominating hydrological processes. In contrast to highly adapted process-oriented models that are based on intensive experimental process investigations (e.g. TAC^D: UHLENBROOK et al. 2004), the model in this study was applied to the upper-mesoscale (BECKER 1992) Fyrisån basin, for which no comprehensive process studies were available. Consequently the focus of this study was to design a runoff generation module that is capable to capture fundamental runoff generation processes sufficiently and concurrently account for the fundamental nitrogen transport processes (cf. 2.1).

In view of this, the standard two-box configuration of the HBV model was chosen as a starting point for further developments. This configuration has been specifically designed for Nordic environments and has proven its applicability and robustness in innumerable applications in Sweden (e.g. BERGSTRÖM 1998; LIDÉN 2000; LINDSTRÖM et al. 1997; SEIBERT 1999a). In addition five runoff generation types were identified reflecting different hydrological and chemical processes in forest, agriculture, wetlands, urban areas and lakes. Their delineation was mainly guided by the assumption that the land use distribution can be seen as a rough surrogate for the allocation of underlying soil types (cf. 3) controlling runoff formation and nitrogen transport processes. Consequently each runoff generation type is assigned to a specific linear reservoir configuration and is parameterised individually. In the following section the different runoff generation types are described in more detail.

Forest, Agriculture and Urban

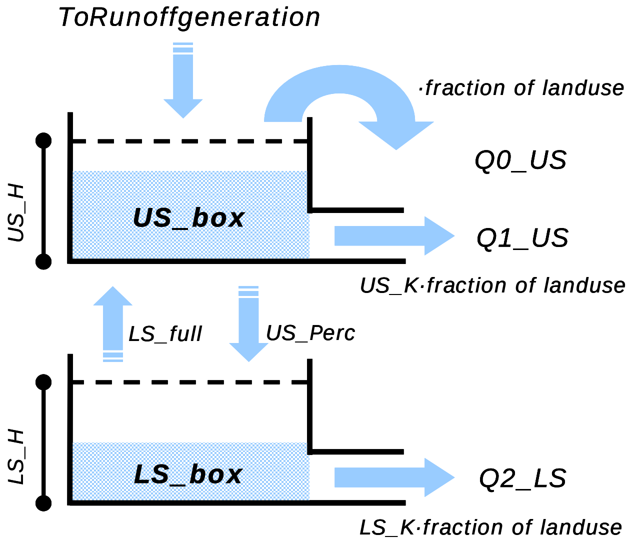

Figure 4.6: Single reservoir configuration and parameterisation of the runoff generation types forest, agriculture and urban.

The runoff generation types forest, agriculture and urban share the same linear storage concept, but are parameterised individually. The configuration of storage boxes is similar to the standard HBV model and consist of an upper linear (*US_box*) and one lower linear storage box (*LS_box*) representing the origin of quick and slow runoff components. Percolation of excess water from the soil routine contributes to the upper storage (*ToRunoffgeneration*) and results in further percolation down to the lower storage box based on the parameter *US_PERC*. If the yield from the soil routine exceeds the percolation capacity, discharge is generated from the upper storage box according to the recession coefficient (*US_K*) and the fraction of land use type (*fraction of landuse*) which implements the sub-grid parameterisation scheme (cf. 4.2.7):

$$Q1\_US = US\_box \cdot US\_K \cdot fraction\ of\ landuse \qquad \textbf{Eq. 4.11}$$

Q1_US:	Runoff component from upper zone (mm d^{-1})
US_box:	Storage in upper zone (mm)
US_K:	Recession coefficient for upper zone (d^{-1})
fraction of landuse:	Fraction of land use according to sub-grid parameterisation (-)

The conceptualisation of the upper reservoir represents the lumped effect of sub-surface runoff generation processes that contribute to faster runoff components in the hydrograph, such as drainage through superficial channels. If a threshold (*US_H*) is exceeded, overflow is enabled (*Q0_US*) and contributes to the fast runoff component. This implementation of overland flow was not necessary from a process realistic standpoint, since overland flow in Sweden is hardly achieved due to highly pervious soils in combination with moderate rainfall intensities (BERGSTRÖM 1976). O^{18} studies showed that river runoff is usually dominated by subsurface flow in Sweden (e.g. RODHE 1987). Nevertheless the description of overland flow was included to avoid high unnatural storage amounts in drainage cells situated at the end of several interconnected storage cascades.

In contrast to the upper storage box the lower storage represents the groundwater storage of the catchment and constitutes the base flow:

$$Q2\_LS = LS\_box \cdot LS\_K \cdot \text{fraction of land use} \qquad \textbf{Eq. 4.12}$$

Q2_LS:	Runoff component from lower zone (mm d^{-1})
LS_box:	Storage in lower zone (mm)
LS_K:	Recession coefficient for lower zone (d^{-1})
fraction of land use:	Fraction of land use according to sub-grid parameterisation (-)

If a threshold (*LS_H*) is exceeded, the excess water contributes to the upper storage (*LS_full)* simulating a raise of the groundwater table. This configuration of the linear storage is parameterised individually per runoff generation type. Due to the fact that an automatic parameterisation estimator was employed in this study, the choice of initial parameters was preliminary and guided by basic assumptions about the hydrologic processes in each land use class. A more damped runoff characteristic with lower recession coefficients than agriculture and settlements was assumed for forested areas, as forest also may contribute more to constant base flow during flow recession. With regard to settlements, quick urban runoff components were already accounted for in the urban runoff routine. Hence, for subsequent runoff generation recession coefficients closer to agriculture were chosen for the initialisation with respect to the rural character of many settlements within the drainage basin. In terms of nitrogen transport this assumption was regarded sufficient as forest areas tend to retain nitrogen in contrast to the more intense nitrogen leaching of agricultural and urban areas.

Wetland

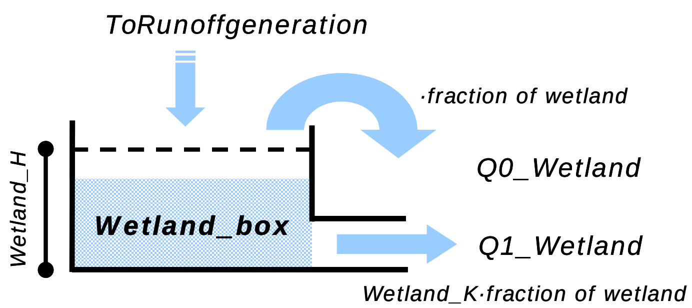

Figure 4.7: Single reservoir configuration and parameterisation of the runoff generation type wetland.

Besides the two-box concept a single linear reservoir storages concept was introduced for the runoff generation type of wetland. It corresponds in its concept to the upper storage box of the two-box concept and is also weighted according to the sub-grid parameterisation scheme by *fraction of wetland* (cf. 4.2.7). During initial parameterisation relative low recession constants were assigned as wetland areas may be characterised by comparatively high storage amounts and a constant contribution to base flow (e.g. BRANDESTEN 1987). With respect to nitrogen retention wetlands are assumed to play a key role to retain nitrogen and therewith small recession coefficients seem to be an adequate representation (e.g. RAISIN & MITCHELL 1995).

Lake

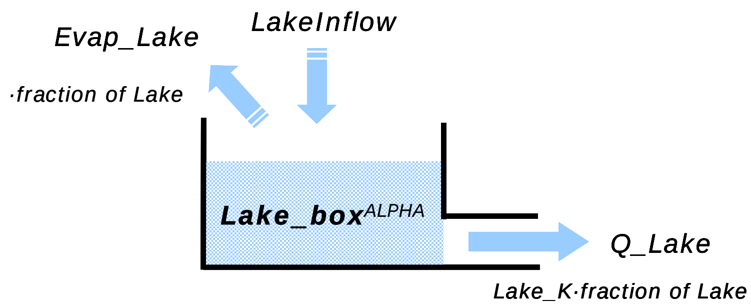

Figure 4.8: Single non-linear reservoir configuration and parameterisation of the runoff generation type lake.

A key element of the model structure in this study is the inclusion of lakes. The role of lakes in the model concept is twofold. On the one hand lakes are linked to the runoff generation routine by being laterally interconnected to the adjacent runoff generation types. On the other hand they are an integral component of the routing routine by interconnecting streams and simulating retention processes. Lake retention and routing in conceptual models is often realised by simple power and polynomial functions (e.g. KOUWEN 2000). These are mostly adapted to available storage-discharge curves at the lake outlet or standard rating curves for specific lake characteristics are available. In the Fyrisån basin such data was lacking. Thus, lake routing is achieved by conceptualising the lakes as a non-linear storage function that is subject to calibration:

$$Q\_Lake = Lake\_K \cdot fraction\ of\ Lake \cdot Lake\_box^{ALPHA} \qquad \textbf{Eq. 4.13}$$

Q_Lake:	Runoff at lake outlet (mm d^{-1})
Lake_box:	Storage in lake (mm)
ALPHA:	Non linear storage coefficient (-)
Lake_K:	Recession coefficient for lake outflow (d^{-1})
fraction of lake:	Fraction of lake according to sub-grid parameterisation (-)

Hence lake outflow and therewith lake routing and retention is controlled by the parameter *LS_K* and *ALPHA*. It is weighted according to the contribution of lake to each grid cell with *fraction of lake*. Moreover potential evaporation from the open surface water table is enabled. The choice of initial parameter for the lake runoff generation type was guided by the assumption that the water residence time in the major lakes in the catchment is not very high (e.g. BRUNBERG & BLOMQVIST 1998), as most lakes are quite shallow and therefore relatively high initial parameter values for the lake routine were assumed.

Lateral flows

Lateral connection of the different runoff generation types within the model is enabled by the local drain direction network (LDD) on a grid cell level, according to the steepest slope between grid cells (cf. 4.2.1). Figure 4.9 gives an overview of the lateral connection between each runoff generation type. Agriculture, forest and urban runoff generation types share the same single reservoir storage configuration and their respective upper storages as well as and lower storages drain into each other if they are situated on a downstream cell. If a wetland runoff generation type holds this position, both runoff components are summed and added to the single wetland storage, while the wetland runoff component is always directed to the upper storage box of potential downstream runoff generation types. If a cell is identified as stream or lake grid cell all runoff is directed to them and no further lateral movement, besides the river and lake routing is possible.

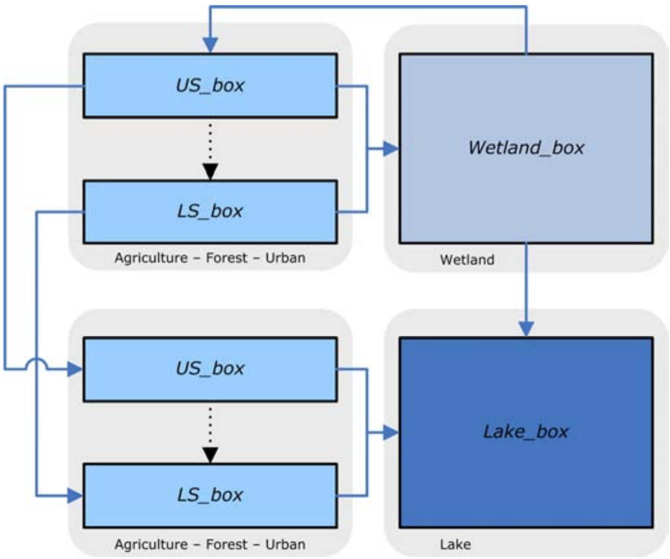

Figure 4.9: Overview of lateral connections (solid arrows) and vertical fluxes (dotted arrows) of the runoff generation types used in the model (after KONZ 2005).

4.2.7. Sub-grid variability

One of the core elements of the developed hydrologic model is the consideration of sub-grid scale variability of land use distribution within the Fyrisån catchment. Therefore a new sub-grid parameterisation scheme was introduced that incorporates land use allocation within a single grid cell. Its implementation is ensured on a sub-grid level by introducing each land use class as a fraction of surface layer per grid cell as proposed by BECKER & BRAUN (1999). Consequently the sum of all land use surface fractions equals the surface area of one cell. In the present model five land use classes (forest, agriculture, urban area, lakes and wetlands) are differentiated and each is assigned to a specific parameterised and designed runoff generation routine utilising the linear storage analogy concept. These designated fractions are than used to weight flow and storage amounts for each associated runoff generation class in order to ensure realistic mean flow and storage conditions for the whole grid cell. Figure 4.10 illustrates the model structure and all underlying model operations within a single grid cell according to their respective contribution of land use class. Lateral cell to cell processes include flows and runoff proportions from upper and lower storages as well as channel routing. Vertical processes contain the propagation of water through the different model routines and evapotranspiration from soils, streams and lakes.

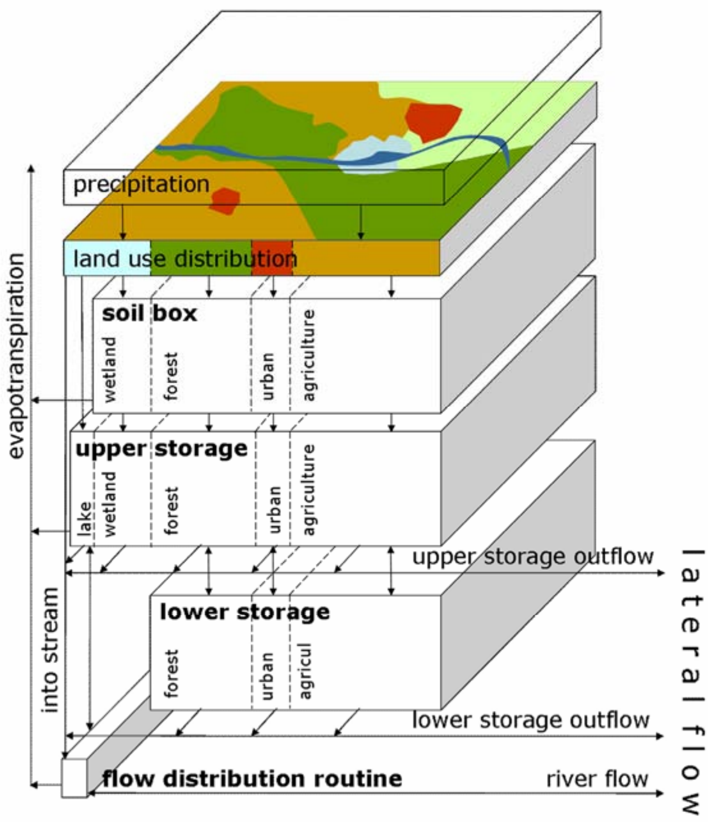

Figure 4.10: Sub-grid parameterisation of the developed distributed model. All water flows and storage within the model routines are weighted according to the designated land use class.

The advantages and applicability of a sub-grid parameterisation scheme over conventional grid cell spacing is manifold. In particular it gets effective when the model grid cell resolution exceeds resolution of comparatively smaller scale land use patterns or landscape features. As a result an accurate representation of these patterns is no longer feasible. A conventional procedure to counteract this problem consists in the overall increase of grid cells. But this is only a partial solution as a correct representation of small scale features in most cases can be only achieved with relatively high grid cell resolutions and therefore results in a considerably rise of model computation time. STRASSER & ETCHEVERS (2005) provide an example that necessitated an grid cell increase in resolution of elevation and meteorological input data by factor 64 to improve variability of snowmelt in model simulations. They argued that sub-grid parameterisation methods are beneficial in order to achieve reasonable computation time and data requirements. Certainly a sub-grid parameterisation scheme has clear advantages. Computation might be also increased, but it is only dependent on the number of land use classes or landscape features, as these can be then associated with a specific parameterised runoff generation routine like in the distributed HBV model. Moreover a sub-grid parameterisation is area accurate meaning that the grid resolution has no effect on the correct representation of surface area fractions. Table 4.1 demonstrates the effect of different grid cell resolutions on the distribution of land use in comparison with the distribution obtained by the sub-grid parameterisation scheme for the Fyrisån catchment. It is clearly shown that the latter results in the same land use distribution as the original data set. On the contrary conventional grid aggregation which naturally considers only dominant land use characteristics, leads to an overall increase of catchment size and to a substantial decrease of small scale landscape features as illustrated by the almost halved wetland area. The increase of catchment area can be explained by a persistent excess of the real catchment boundary by the coarse raster structure, while the respectively small wetland surface is simply neglected against the predominating and thus growing forest area during grid aggregation.

Table 4.1: Land use distribution of the Fyrisån catchment depending on grid cell resolution.

Land use	Original data set (25 × 25 m²) and sub-grid parameterisation (250 × 250 m²)		Conventional aggregation (250 × 250 m²)	
	km²	%	km²	% of original
Catchment size	2006	100	2063	102.9
Forest	1202	59.9	1303	108.4
Agriculture	646	32.2	638	98.8
Wetlands	91	4.5	57	62.6
Settlements	34	1.7	35	102.9
Lakes	32	1.6	31	96.9

4.2.8. Channel routing and lakes

In distributed hydrologic modelling the flow routing in the channel network is an essential part when considering time series of flows in larger scale model applications. Due to the lack of detailed channel data in combination with numerous lakes and wetlands as well as the flat topography of the territory, it was not possible to use conventional routing methods, such as the kinematic wave approach applied by the TAC^{D} model (UHLENBROOK et al. 2004). Also the application of much simpler techniques like the MAXBAS weighting function of the HBV model was neglected to favour an incorporation of solute transport. A simple method was needed that accounts for both the spatial and temporal distribution of water flow within the channel network. Therefore a relatively simple routing module was developed that computes a downstream distribution according to a parameterised weighting function for the water content of each grid cell within the stream network.

Consequently water fractions of a starting stream cell are distributed over its adjacent downstream cells. The form of the weighting function is dependent on the parameters DMAX (-) and DPEAK (-). DMAX specifies the number of downstream cells over which the water content of the initial cell spreads, while DPEAK is a measure for the location of the maximum peak of the triangular weighting function as shown in Figure 4.11. A daily implementation of the spatial distribution function ensures temporal propagation of water flow. This channel flow is interrupted by numerous lakes in which flow retention occur. Hence stream routing in the model concept is intermitted at lake inlets, and daily stream discharge at these points supplies the lake storage. Moreover lateral flows of adjacent land use cells are also contributing. At the respective lake outlet, outflow is computed on the basis of non-linear storage equations depending on inflow and water storage (cf. 4.2.6.). Afterwards it is added to the next stream section, where the downstream distribution of flow continues. Due to this implementation of the lake and flow routine in combination with spatial representation of lakes throughout the catchment a more process realistic conceptualisation of lake retention and storage can be achieved.

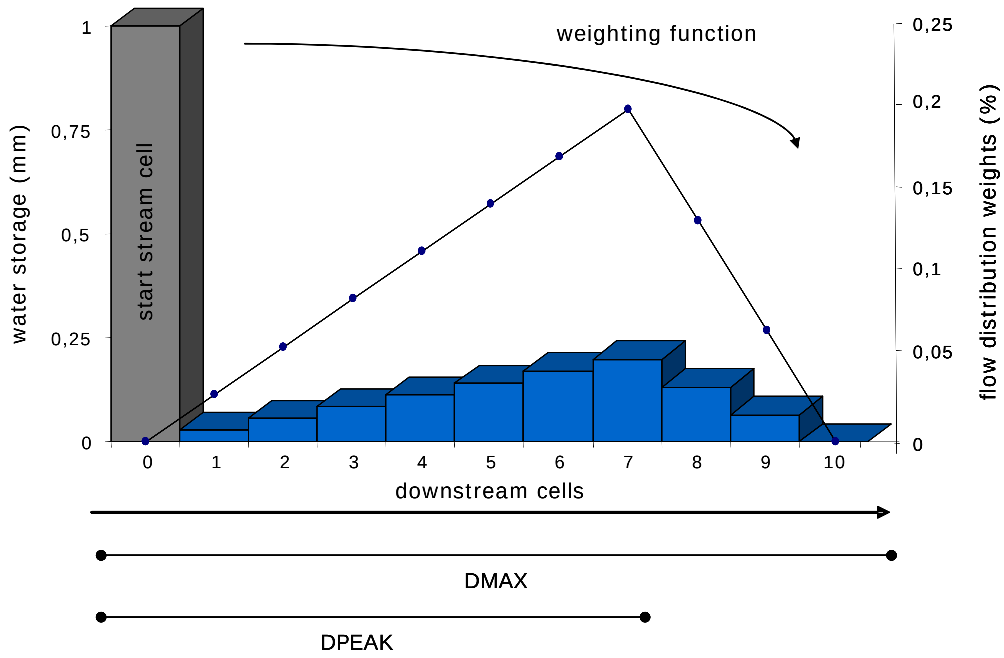

Figure 4.11: Downstream distribution of stream water influenced by the flow distribution parameters DMAX and DPEAK.

4.2.9. Water management

The Fyrisån is subject to regulation by artificial stream water withdrawal as well as additional water transfer to the catchment. Daily time series were available for the water transfer from lake Tämnaren outside the catchment to the Fyrisån as well as for water withdrawal from the stream. A simple water management routine was implemented accounting for these effects by adding, removing or transferring the respective amount of water to the stream at distinct key grid cells.

4.2.10. Run-time performance enhancements of the model

In general, the run-time performance of the hydrological model with linked solute transport routines was rather poor and resulted for example in a six hour model run for the period 1998 to 2005. This might be not important for single model runs, but as soon as calibration is involved the number of necessary model runs increases considerably and calls for efficient run-time performance enhancements. Especially the coupling with the automated parameter estimation programme PEST required extensive model runs depending on the amount of parameters involved. Different modifications of the model code were necessary to enhance the performance of the model simulation. A careful revision of the source code was necessary to ensure a most efficient implementation of the model routines. The introduction of fixed inverse distance weights and the use of maps that represented the extent of catchments and sub-catchments most exactly in terms of the rectangular-shape of base maps stored by

PCRaster reduced the amount of missing values notably and led to an overall gain in performance.

4.2.11. Verification

A measure for model verification during model development was the implementation of a test site. A virtual test site is a small representation of the catchment with the same features as the real catchment model in order to support model development and subroutine testing within a manageable area in connection with short computation times. Thus the test area helped to identify potential source code errors and played an important role in optimising the model source code.

One of the main criterions helping to verify the correctness of a rainfall-runoff model is its internal water balance. The internal water balance computes the sum of all input- and output-fluxes as well as the water level of all storages within the model for each time step and provides a diagnostic test for the violation of mass conservation within the model structure (WISSMEIER 2005). In the present model version the internal water balance includes precipitation and artificial water transfer into the catchment as input quantities, as output quantities river flow at the catchment outlet and losses due to evaporation are considered. Initial and end storages are taken into account comprising snowpack, water content of the snowpack, soil moisture, water level of upper and lower storage boxes as well as water distribution within the stream network. Due to the integrative character of the internal water balance it proofed to be a helpful tool in the course of the model development to quickly check for fundamental errors in the model source code. Consequently a correct internal water balance is the fundamental prerequisite for a further model application after completed model development. However, a correct water balance does not necessarily guarantee an error free source code. The model verification within this thesis revealed a stable cumulated water balance for the entire model application period of the developed hydrological model.

4.2.12. Parameterisation

For the automatic model calibration 19 of the most essential model parameters out of 28 were selected. The remaining parameters were fixed according to literature values or tied with a certain ratio to parameters that were subject to the calibration process in order to reduce the overall parameter space and enable a fast and successful calibration result. Table 4.2 gives an overview of the model parameters. For each parameter a variation range or search space was defined by setting an upper and lower bound. These parameter limits were specified according to previous HBV model applications (e.g. BERGSTRÖM 1990; SEIBERT 1999b) as well as TAC^D model applications (e.g. UHLENBROOK et al. 2004) and depend on the physical and mathematical constrains of the model. Initial parameter values were selected on the basis of previous best manual calibration trials in order to start with the optimal known parameter set. By choosing these initial parameter sets from different ranges within the parameter space, the capability of PEST to find the global minimum over local minima of the objective function was determined.

Table 4.2: Model parameters with ranges and initial values used for the PEST calibration of the hydrological model.

Parameter	Explanation	Unit	Initial	Minimum	Maximum	Estimate
Snow routine						
TT	Threshold temperature	°C	0	-2.5	2.5	calibrated
TT_{diff}	TT for forest	°C	0	-2.5	2.5	calibrated
SFCF	Snowfall correction factor	-	0.6	0.4	1	calibrated
$SFCF_{diff}$	SFCF for forest	-	0	0.4	1	calibrated
CFMAX	Degree-day factor	mm °C^{-1} d^{-1}	2	1	8	calibrated
CWH	Water holding capacity	-	0.1	-	-	fixed[a]
CFR	Refreezing coefficient	-	0.05	-	-	fixed[a]
Soil routine						
LP	Reduction of evaporation	-	0.6	0.3	1	calibrated
FC_{forest}	Field capacity for forest	mm	300	50	500	calibrated
$FC_{agricul}$	Field capacity for agriculture	mm	200	50	500	calibrated
$FC_{wetland}$	Field capacity for wetland	mm	100	-	-	tied
FC_{urban}	Field capacity for urban	mm	150	-	-	tied
$BETA_{forest}$	Shape coefficient for forest	-	4	1	6	calibrated
$BETA_{agricul}$	Shape coefficient for agriculture	-	4	-	-	tied
$BETA_{wetland}$	Shape coefficient for wetland	-	4	-	-	tied
$BETA_{urban}$	Shape coefficient for urban	-	4	-	-	tied
Runoff generation routine						
UrbanSplit	Portion of sealed urban areas	d^{-1}	0.5	-	-	fixed
$K_{US\ forest}$	Upper recession coefficient for forest	d^{-1}	0.25	0.01	0.4	calibrated
$K_{LS\ forest}$	Lower recession coefficient for forest	d^{-1}	0.005	0.001	0.15	calibrated
$PERC_{forest}$	Percolation from upper to lower box forest	mm d^{-1}	0.05	0.001	3	calibrated
$H_{US\ forest}$	Maximal storage capacity upper box forest	mm	350	1	1000	calibrated
$H_{LS\ forest}$	Minimal storage capacity lower box forest	mm	1000	-	-	fixed
$K_{US\ agricul}$	Upper recession coefficient for agriculture	d^{-1}	0.35	0.01	0.4	calibrated
$K_{LS\ agricul}$	Lower recession coefficient for agriculture	d^{-1}	0.007	0.001	0.15	calibrated
$PERC_{agricul}$	Percolation from upper to lower box agricul.	mm d^{-1}	0.008	0.001	3	calibrated
$H_{US\ agricul}$	Maximal storage capacity upper box agricul.	mm d^{-1}	250	1	1000	calibrated
$H_{LS\ agricul}$	Minimal storage capacity lower box agricul.	mm d^{-1}	1000	-	-	fixed
$K_{US\ wetland}$	Upper recession coefficient for wetland	d^{-1}	0.05	0.01	0.4	calibrated
$H_{US\ wetland}$	Maximal storage capacity upper box wetl.	mm d^{-1}	150	-	-	calibrated
$K_{US\ urban}$	Upper recession coefficient for urban	d^{-1}	0.5	0.01	0.4	calibrated
$K_{LS\ urban}$	Lower recession coefficient for urban	d^{-1}	0.003	0.001	0.15	calibrated
$PERC_{urban}$	Percolation from upper to lower box urban	mm d^{-1}	0.01	0.001	3	calibrated
$H_{US\ urban}$	Maximal storage capacity upper box urban	mm d^{-1}	100	1	1000	calibrated
$H_{LS\ urban}$	Minimal storage capacity lower box urban	mm d^{-1}	1000	-	-	fixed
Lake and flow distribution routine						
K_{lake}	Recession coefficient lake	d^{-1}	1	0.001	1	calibrated
$ALPHA_{lake}$	Nonlinear weighting coefficient lake	-	1	0.001	1	calibrated
DMAX	Flow distribution length	-	109.1	3	160	calibrated
PEAK	Flow distribution peak location	-	81.83	-	-	tied

[a] BERGSTRÖM (1992)

4.2.13. Evaluation model and objective functions

According to the work of WISSMEIER (2005) an external evaluation model was written and coupled to the hydrologic model. Objective functions are computed by the evaluation model immediately after the main hydrologic model completed its run. In combination with the automated parameter estimator PEST, the evaluation model provides the objective function that is subject to the optimisation procedure. To evaluate the goodness of the obtained parameter sets in the course of the automatic calibration process, different objective functions were used, as they judge the model performance by different aspects (SEIBERT 1999b). In addition to the traditional R_{eff} and V_E criterions (Table 4.3) (NASH & SUTCLIFFE 1970), the R_V criterion proposed by LINDSTRÖM ET AL. (1997) was finally chosen for the model calibration procedure, as it proved to be a good compromise between the traditional efficiency R_{eff} and the relative volume error V_E. The R_V produced almost as high R_{eff} values with a significantly reduced volume error V_E for prior lumped HBV model applications (LINDSTRÖM et al. 1997).

Table 4.3: Objective functions used for the model evaluation.

Objective function	Symbol	Definition	Unit	Value for "perfect" fit
Efficiency[a]	R_{eff}	$1-\frac{\sum_{i=1}^{n}\left(Q_{i,obs}-Q_{i,sim}\right)^2}{\sum_{i=1}^{n}\left(Q_{i,obs}-\overline{Q_{obs}}\right)^2}$	-	1
Relative volume error	V_E	$\frac{\sum_{i=1}^{n}\left(Q_{i,obs}-Q_{i,sim}\right)}{\sum_{i=1}^{n}Q_{i,obs}}$	-	0
R_V criterion[b]	R_v	$R_{eff}-w\cdot\lvert V_E\rvert$	-	1

[a] NASH & SUTCLIFFE (1970); [b] LINDSTRÖM et al. (1997) with weight: $w = 0.1$

4.3. Solute transport model

4.3.1. Basic model concept

Modelling of nitrogen in a conceptual way is principally based on routing the nitrogen load from the source to the catchment outlet. For this purpose the distributed hydrologic model was equipped with solute transport routines to allow the simulation of nitrogen transport and transformation at the catchment-scale. The solute transport model is directly linked to the underlying distributed hydrologic model using its water fluxes and storage levels to route nitrogen through the routines of the catchment model. A consistent implementation of the solute transport routine is achieved by a parallel system of distributed storages analogue to the hydrologic model structure that enables advective solute transport and mixing in all sections. The transport model is based on the model extension for solute transport of the TAC^D model and was developed by WISSMEIER (2005). Since this extension allows only conservative solute transport, further conceptualisations regarding nitrogen turn over process in soils and retention in water courses were necessary. Terrestrial leakage of nitrogen was included implicitly in the model by applying a standard leakage coefficient methodology (e.g. BRANDT et al. 2002). This technique is based on nitrogen transport simulations of the one-dimensional physically based SOILNDB model which was applied for various combinations of crop, soil type, and agricultural management practice as well as climate conditions in Sweden. The resulting standard leaching coefficients describe leakage of nitrogen into the runoff response unit of the model depending on simulated groundwater recharge. Nitrogen retention in groundwater, rivers and lakes is accounted for by parameterised retention functions according to concepts of the HBV-N model (e.g. ARHEIMER 1998). With these conceptualisations and the appropriate input data the model is capable of simulating source and flow processes of point and non-point sources of nitrogen in a fully distributed manner. The schematic structure of the nitrogen transport model and its coupling with the hydrological model is demonstrated in Figure 4.12. A detailed description of the conceptualisation of nitrogen transport, terrestrial leakage, and retention can be found in the subsequent chapters.

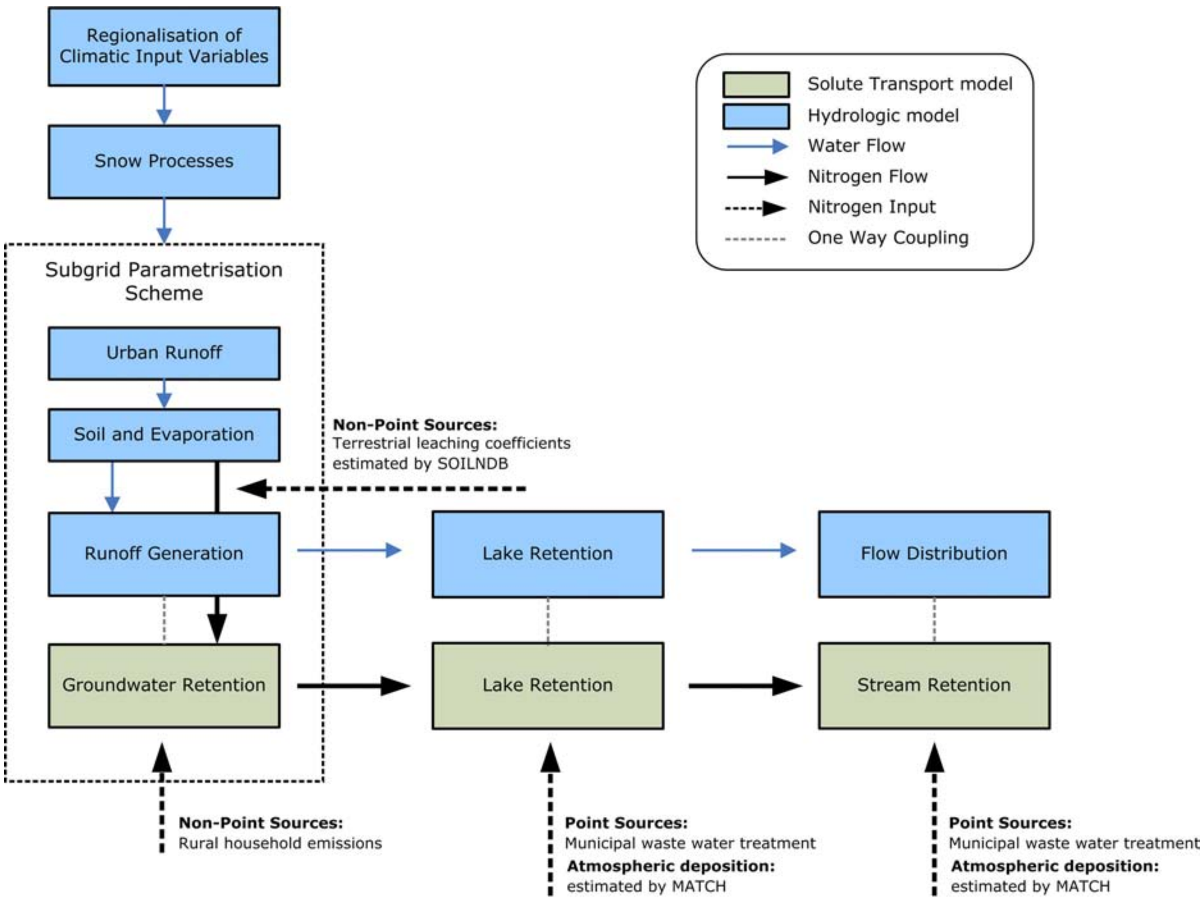

Figure 4.12: Schematic structure of the coupling between hydrologic and nitrogen transport model.

4.3.2. Modelling nitrogen transport

The conceptualisation of nitrogen transport within this model application is based on the work of WISSMEIER (2005) and utilises a parallel architecture of storages for solute transport mirroring the underlying hydrologic model and using its generated flows and storage amounts as driving variables for the nitrogen transport. Concretely, each storage and flux of the hydrologic model has its corresponding storage or flux of solute. Coupling of both models is achieved by interconnecting water fluxes with nitrogen fluxes by the following basic equation:

$$-\frac{dN}{dt} = \frac{Q \cdot N}{V} \qquad \textbf{Eq. 4.14}$$

Q:	Water flux (mm d^{-1})
V:	Volume of water within the water storage (mm)
dN/dt:	Nitrogen flux (mg d^{-1})
N:	Amount of nitrogen within the nitrogen storage (mg)

The parallel architecture of the model becomes more obvious if

$$-\frac{dV}{dt} = Q \qquad \textbf{Eq. 4.15}$$

is introduced and combined with equation 4.15, resulting in following expression:

$$\frac{dN}{N \cdot dt} = \frac{dV}{V \cdot dt} \qquad \textbf{Eq. 4.16}$$

These equations show that processes within the solute model depend only on parameterisation of the hydrologic model, if no further retention or nitrogen degradation functions are applied. Thus the quality of nitrogen model simulations depends mainly on the correct representation of water fluxes and storages by the hydrologic model, as storage volumes determine the degree of dilution of nitrogen and parameterisation of water flux affects nitrogen transport accordingly. Simulations of nitrogen transport can therefore be a valuable tool in terms of multi-criteria calibration and validation and furthermore can help to detect inadequate model formulations.

In this regard water residence time is an additional factor controlling nitrogen transport, since it has major effect on the biological transformation of nitrogen so that longer hydrological residence times result in an increased reduction of nitrogen from the water phase. Inside the model structure residence time is implicitly addressed by the hydrological response routine describing water storages in conjunction with the lateral alignment of storage boxes. This allows depending on the spatial situation, the formation of storage cascades which may results in a subsequent translation and dispersion of the nitrogen concentration.

Transport routines were implemented in the existing structure of the hydrological model starting from the runoff generation routine onwards. No additional incorporation of model routines was needed, as in-soil processes of nitrogen transformation comprise atmospheric deposition by applying a long-term leaching coefficient methodology (cf. 4.3.3). Nitrogen transport modelling starts with the input of diffuse sources by terrestrial leakage and rural household emissions in the runoff generation routine. The nitrogen concentrations are computed by the model and atmospheric nitrogen deposition on open watercourses and point emissions of municipal water treatment plants into streams are added subsequently. During these inputs mixing of different nitrogen concentration is simulated dynamically on the way downstream by the model in each grid cell, while nitrogen retention is applied for groundwater, lakes, and streams. Nitrogen transport is calculated by the model as specific nitrogen load. Point and non-point input data can be provided in *mg/m²* or *mg/l* and are transformed into specific loads afterwards. Concentration values of nitrogen can be easily obtained in the course of the model simulation for each grid cell and time step by dividing the mass of nitrogen by the associated water volume of the underlying hydrologic model.

4.3.3. Modelling terrestrial leakage

Diffuse nitrogen pollution from agricultural land is one of the major contributors to nitrogen loads in fresh water bodies. A common approach in nutrient transport modelling is to quantify inputs of diffuse sources and point sources and use them as model inputs. As surface nitrogen loss through arable field erosion is not significant (e.g. HARALDSEN et al. 1995), diffuse soil losses can be described by root zone leakage alone. While empirical measurements are in most cases related to the plot scale and long time series are not often available, nitrogen leaching models offer the possibility to derive leakage concentrations based on a detailed description of physiography and land management.

A frequently used model in Scandinavia to asses nitrogen leaching from soils is the SOILNDB model (JOHNSON et al. 2002). SOILNDB is a one-dimensional model simulating nitrogen dynamics and losses in soil profiles of arable land. It links input data and data from parameter data bases to automatic parameterisation procedures for two underlying physically-based models: a soil nitrogen model SOILN (JOHNSSON et al. 1987) and a water and heat model SOIL (JANSSON & HALLDIN 1979). While the SOIL model provides the driving variables for the SOILN model, SOILN includes all major processes determining transport and transformation of nitrogen in arable soils. In detail the SOIL model includes snow dynamics, frost, evapotranspiration, infiltration, surface runoff, drainage flows, and water uptake by vegetation. Water flow between soil layers is described by Darcy’s law and by preservation of water balance whereas heat flow follows Fourier based rules. In the SOILN model nitrogen is divided into inorganic nitrogen in the form of NO_3^- and NH_4^+, and three organic nitrogen pools: a litter pool consisting of microbes and fresh organic material such as decomposing roots, a humus pool comprising more stable organic matter, and a faeces pool containing added manure. Following processes are included: mineralisation dependent on soil temperature and moisture, decomposition to CO_2, humus and recycling within the pool, soil temperature function, plant uptake from empirical functions, denitrification dependent on soil temperature, soil oxygen status and soil nitrate content. Inputs of nitrogen can be applied in the form of fertiliser, manure, and atmospheric deposition. Harvested crop, leaching, and denitrification constitute to the model output.

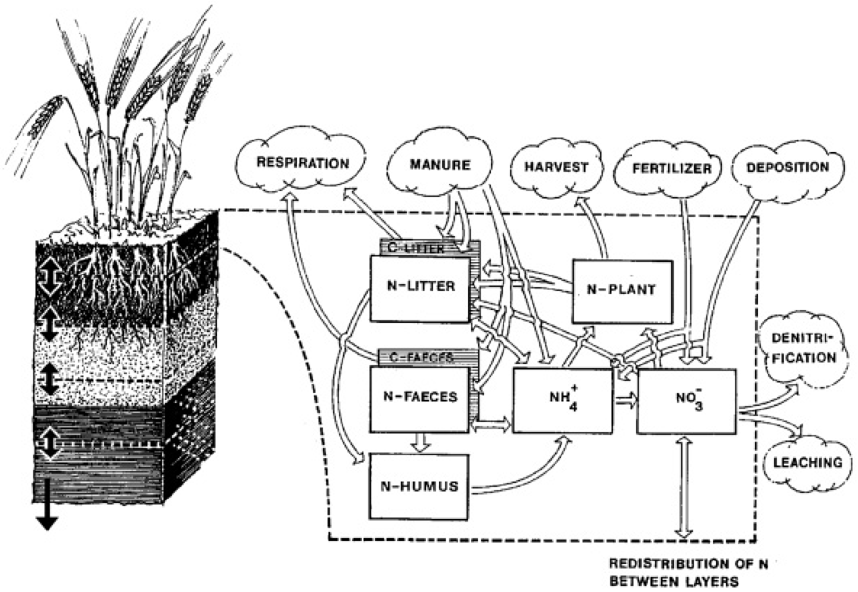

Figure 4.13: Schematic structure of the SOIL-N model (from BRANDT et al. 2002).

SOIL and SOILN have been used in many studies mainly at field scales (e.g. HOFFMANN & JOHNSSON 2003), but have been also linked to catchment-scale hydrological models, such as HBV-N (e.g. ARHEIMER & BRANDT 1998). Within the TRK project (BRANDT et al. 2002; JOHNSSON et al. 2002) the model was applied for a combination of cropping situations, soil types, and climate regions in Sweden. Long term averages of nitrogen leakage within the root-zone at a depth of one meter below soil surface were the result. The main advantage of implementing these standard leaching coefficients in catchment-scale nitrogen models is the inclusion of top soil processes such as denitrification so that the nitrogen content can further leak into the ground or move along with the groundwater and reach surface water bodies.

To achieve temporal variable nitrogen root zone concentrations the hydrologic model provides dynamically simulated groundwater recharge as driving variable. Leakage occurs only if the groundwater recharge is larger than zero. In this case the standard leakage coefficients are multiplied with the simulated daily recharge and the resulting specific nitrogen load is added to the pool in the runoff response routine. Thus temporal and spatial variability of nitrogen leakage as well as transformation of nitrogen in the saturated and unsaturated zone can be considered implicitly, while the model has to account explicitly for retention in ground and surface waters as pointed out in the next section.

4.3.4. Modelling retention

Nitrogen retention can be defined as the net effect of various biogeochemical processes, such as biological uptake (assimilation) and definite nutrient removal from the water phase by sedimentation and denitrification (e.g. ANDERSSON et al. 2005). Various methods exist to account for nitrogen retention in conceptual models. For the actual model development different conceptual measures and functions for riverine retention have been reviewed ranging from very simple retention factors (e.g. KVARNÄS 1996) and exponential equations (e.g. ALEXANDER et al. 2000; DE WIT 2001) to more complex conceptual assumptions (e.g. KRYSANOVA & BECKER 1999).

The simple approach used in the HBV-N model (ARHEIMER 1998) was regarded as most suitable for the implementation of retention in this study, as it was frequently applied for nitrogen transport studies under Nordic conditions in Scandinavia and revealed in most cases adequate results with comparatively little parameterisation effort.

Consequently the retention function was integrated in the model structure, but was subject to modifications in order to meet the distributed model requirements. On the one hand an implementation per grid cell was necessary in contrast to the application to sub-catchments in the semi distributed HBV-N model, while on the other hand the distinction between inorganic and organic nitrogen fraction was removed to reduce the data demand of the model. The lumped effect of Tot-N retention is expressed by the model equations which are mainly dominated by the inorganic fraction in Nordic environments. As a result, concentration dynamics for nitrogen are computed for each grid cell by following fundamental equation:

$$\frac{d(c \cdot V)}{dt} = c_{in} \cdot Q_{in} + P + D - \phi - c \cdot Q_{out} \qquad \textbf{Eq. 4.17}$$

c:	Tot-N nitrogen concentration (mg mm^{-2} d^{-1})
V:	Water volume of response box, river or lake (mm d^{-1})
c_{in}:	Inflow concentration (mg mm^{-2} d^{-1})
Q_{in}:	Runoff inflow (mm d^{-1})
t:	Time (day)
P:	Point Source (mg d^{-1})
D:	Atmospheric deposition on open water bodies (mg d^{-1})
ϕ:	Lumped effect of biochemical transformation (mg d^{-1})
Q_{out}:	Runoff outflow (mm d^{-1})

In this equation ϕ is a function representing the lumped effect of retention and is varied for different freshwater bodies. It is based on empirical relationships between physical variables, landscape characteristics, and concentration dynamics reflecting the net reduction by turnover processes. Turnover processes affect nitrogen loads during residence in the different water bodies of groundwaters, streams, and lakes (Table 4.4).

Table 4.4: Retention expressions of different water storages used in the solute transport model (from ARHEIMER 1998).

Water Storage	ϕ [a] in Equation Eq. 4.19	Abbreviations
Groundwater	$k_{Groundwater} \cdot T_{10} \cdot c \cdot Q$	*k:* Calibration parameter
		T_{10}: 10-day-mean air temperature
Lake	$k_{Lake} \cdot T_{10} \cdot c \cdot Q \cdot A_{Lake}$	*c:* Concentration
River	$k_{River} \cdot T_{10} \cdot c \cdot Q$	*Q:* Runoff

[a] $\phi = 0$ if temperature T_{10} drops below 0 °C

As it can be seen, ϕ is mainly dependent on temperature and nitrogen concentration and includes parameters that can be calibrated against temporal and spatial observations of nutrient concentrations. The underlying assumptions are that denitrification and plant uptake are major processes for nitrogen retention and that both are correlated to air temperature. According to LIDÈN (2000) these assumptions are valid, since a direct relation between temperature in water and in soil has been proved (e.g. SEITZINGER 1988). Moreover empirical findings in small forest streams in Scandinavia indicate that the plant growth season is in Nordic climate is closely linked to the temperature cycle of the year (e.g. ARHEIMER et al. 1996). To account for the delay between temperature in soil and water compared to air temperature, it is common practice in the HBV-N model application to use a 10-day running mean of the areal air temperature in the basin. For lakes an additional factor of lake surface area is introduced following the idea that denitrification is the major sink in lakes and occurs mainly at the sediment-water interface. At temperatures below zero biogeochemical processes are neglected and retention is not simulated by the model equations. In general a robust method with little parameterisation demand was introduced that accounts for variable retention in different surface water bodies based on empirical relations.

4.3.5. Verification

Different tests were performed to approve the correct implementation of the nitrogen transport model and its coupling to the hydrological model. Equivalent to the water balance the internal solute balance was used as a main criterion to verify the source code for fundamental errors during model development. A stable cumulated internal solute balance could be derived for the application period 1999 to 2005 as a prerequisite for further model applications.

In addition, test procedures proposed from WISSMEIER (2005) were carried out to ensure a correct nutrient transport in different situations without retention effects. The so-called constant concentration test uses the same water and respective nitrogen concentration inputs to the transport model. The same simulated constant concentration levels can be expected as output concentration, if further effects such as evapotranspiration are assumed to affect both water and nitrogen loads in the same kind and retention functions are switched of. A further simple test with synthetic data involved the model reaction to instantaneous point source inputs and instantaneous diffuse source inputs at different locations throughout the catchment.

All aforementioned tests were carried out successfully and confirmed the correct conceptualisation and programming of the nitrogen transport model as a prerequisite for further model applications in this study.

4.3.6. Parameterisation

The automatic calibration of the solute transport module included only three parameters of the retention functions, since the hydrological model was optimised in a separate calibration trial and hydrological driving variables are used for the nitrogen transport simulation. For each parameter a variation range was defined by setting an upper and lower bound. These parameter limits were not specified explicitly, as no experience with this equation for fully distributed concepts existed. Thus parameters were all regarded as free and all had the same weight on the optimisation result derived by PEST.

Table 4.5: Model parameters with ranges and initial values used for the PEST calibration of the solute transport model.

Parameter	Explanation	Unit	Initial	Minimum	Maximum	Estimate
Retention parameters						
$k_{Groundwater}$	Retention factor for Groundwater	-	0.002	0.00001	1	calibrated
k_{Lake}	Retention factor for Lakes	-	0.001	0.00001	1	calibrated
$k_{Wetland}$	Retention factor for Wetlands	-	0.0005	0.00001	1	calibrated

5. Data base

Collection, processing, and allocation of input data in the Fyrisån drainage basin was one major concern besides the model development in this study. The objective was to create a central data base which contains on the one hand all necessary information for the hydrologic and solute transport based model application, and on the other hand provides a basis for future model application in the Fyrisån basin by ensuring easy access to consistent input data.

In the course of the study different institutions and authorities contributed with various spatial and temporal data sets to the model simulation. In particular data collection of emission sources was complicated by the fact that the Fyrisån watershed is part of six different municipalities, all having a different focus and way of data treatment and allocation. This resulted in rather time consuming data collection process, but as a result the most recent and detailed information available was obtained for this catchment. Datasets were provided in different formats as well as spatial and temporal resolutions. Intensive processing of the data was therefore a prerequisite for a successful model application and data base compilation. Spatial data was converted and resampled to grids to correspond to the model resolution of 250×250 m², while temporal records underwent interpolation or aggregation to meet the daily time step of the model. Most data sets were already processed by their home institutions and were checked for integrity and consistency. Hence only additional visual inspection was done during data base compilation.

An overview of all data sets contained in this study can be found in Table 5.1. The subsequent paragraphs give a detailed description of the data processing and analysis that was carried out. Coordinates and additional data for stations discussed in this section can be found in the Appendix.

Table 5.1: Data base of model input data for the application in the Fyrisån catchment.

Data	Resolution/Stations	References
Topography		
DEM	90 × 90 m²	SRTM (2005) / Lantmateriet
Hydrography		
River basins	-	SMHI
River network	1:50 000	TERRÄNGKARTAN (2003)
Lakes	1:50 000	TERRÄNGKARTAN (2003)
Land use		
Forest	1:50 000	TERRÄNGKARTAN (2003)
Agriculture	1:50 000	TERRÄNGKARTAN (2003)
Settlements	1:50 000	TERRÄNGKARTAN (2003)
Wetlands	1:50 000	TERRÄNGKARTAN (2003)
Meteorological data		
Precipitation stations	8 stations	SMHI
Temperature stations	3 stations	SMHI
Potential evaporation	-	ERIKSSON (1981)
Hydrological data		
Discharge stations	3 stations	SMHI
Stream water withdrawal/ groundwater enrichment	1 site	Uppsala komun
Stream water allocation	2 sites	Uppsala komun
*Diffuse Source*s		
Agricultural leaching coefficients	-	IAKS data base with associated TRK leaching coefficients
Atmospheric deposition	30 × 30 km²	MATCH (2005)
Point Sources		
Municipal treatment plant emissions	16 stations	Länsstyrelsen Uppsala
Rural household emissions	> 12000 sites	Länsstyrelsen Uppsala
Chemistry data		
SLU monitoring stations	30 stations	SLU
Synoptic Sampling Campaign	88 sites	cf. 6.

5.1. Spatial data

5.1.1. Digital elevation model

The flatness of the lowland Fyrisån watershed was one main concern during data preparation. For the correct delineation of sub-catchments and the local drainage network a high resolution digital elevation model was necessary. Therefore digital elevation data derived by the Shuttle Radar Topography Mission (SRTM) were applied (e.g. RABUS et al. 2003). These digital elevation models (DEMs) currently available have been processed by the NASA and were derived from interferometric analysis of the C-band signal. The data are grided with a resolution of 3 by 3 arc seconds (SRTM-3) and available for free for most parts of the world (SRTM 2005). Four data sets were used to cover the whole Fyrisån catchment area. After mosaicking the four SRTM DEM files to one and reprojecting the data to the RT90 projection system, several processing steps were necessary including filtering (lowpass and limit filter) as well as filling procedures to obtain a void free and accurate representation of topography. For evaluation purposes the SRTM DEM was compared to a DEM-derived from topographic contours that suffered partly from severe digitalisation errors and thus was not directly applied in this study. The comparison revealed a consistent representation of topography and was considered sufficiently accurate for further practice.

5.1.2. River network and local drainage network

Different vector data sets of the stream network were compared and revealed considerable differences in the representation and connection of river segments as well as major deviations in comparison to topographical maps and DEM-derived topography. The vector layer of stream network of the TERRÄNGKARTAN (2003) was regarded as most sufficient for the representation of the stream network in the Fyrisån catchment. However, it was very detailed and not continuous and needed substantial manual revision. The revision included the removal of small streams and ditches that were considered not important for explicit routing of water by the model as well as the connection of major river segments that were intersected by lakes. The derived sound vector data set was aggregated to the 250×250 m² grid resolution of the model. An aggregation of meandering streams commonly leads to an overestimation of stream cells in the raster format. It was accounted for by a step-wise aggregation procedure starting from higher raster resolutions in combination with the application of a threshold parameter defining the percentage of river area in each grid cell. This procedure allowed to neglect grid cells with low stream percentages. Finally a river network was derived that was considered sufficient for the model application in the Fyrisån basin.

A subsequent delineation of the local drainage network according to the D8 routing algorithm (O'CALLAGHAN & MARK 1984) was based on the derived SRTM DEM. Due to the low relief energy of the region, with predominating flat areas and pits, it was necessary to apply a "stream burning" procedure. This approach was first introduced by HUTCHINSON (1989) and makes use of ancillary information regarding a predefined stream network to force flow through stream cells corresponding to the stream within a DEM-derived local drain direction network. Different values for the stream burning procedure were evaluated and a "burning depth" of 30 m revealed an adequate representation of the "predefined" stream network obtained from the TERRÄNGKARTAN (2003). The derived local drainage direction network enabled lateral routing between the cells.

5.1.3. Land use

Information about land use including stream network and lakes was available as vector data set from respective topographical maps (TERRÄNGKARTAN 2003). Five most characteristic land use classes were identified (forest, agriculture, wetland, settlement, and lake) (Figure 3.1) and re-classification and aggregation of 23 available land use classes to these five classes that were regarded relevant for the hydrological and nutrient transport model application was carried out. To enable sub-grid parameterisation in the model approach, separate maps were produced for each land use class containing an area accurate percentage of a distinct land use type based on the original data set resolution (cf. 4.2.7). In the model concept lakes are conceptualised as single non-linear reservoir storages. To implement this concept in PCRaster, additional lake maps were necessary. Hence a lake classification map was derived by assigning each grid cell belonging to a distinct lake a similar identification number. Additionally, lake in- and outlet points were defined in separate maps in order to facilitate lake in- and outflow and handover of storage outflow or inflow to the adjacent stream network.

5.2. Meteorological and hydrological data

Meteorological and hydrological time series for the investigation period 1992 to 2005 were obtained from the standard observation network of SMHI. Daily uncorrected precipitation data at eight stations situated within the vicinity of the research area and northwards from Uppsala were available. At some precipitation stations shorter gaps in the data records were existent and filled by weighted means of the surrounding stations. Moreover three climate stations that were distributed accordingly provided daily mean temperature data. Regionalisation of meteorological input data was achieved during model application by inverse distance weighting. ERIKSSON (1981) published monthly evapotranspiration estimates for whole Sweden from which suitable values for the Fyrisån catchment were selected. The hydrological discharge-observation network from SMHI contained three regular stations within the drainage basin (Figure 5.1), but no outlet station capturing the total drainage basin was available. The sub-catchments Vattholma and Sävja had continuous records over the whole application period, while for the station of Ulva Kvarn (including the smaller Vattholma sub-catchment) only discharge measurements until the year 2000 were existent. SMHI checked runoff records for consistency and interpolated existing gaps.

Besides these data of the standard hydrological and climatological observation network, additional information about water regulation was available. The data contained time series of water volumes for the time period 1992 to 2003 that were transferred from Lake Tämnaren outside the catchment to the Fyrisån as well as time-series of water volumes that were taken from the Fyrisån and infiltrated artificially in the Uppsala-esker for water supply.

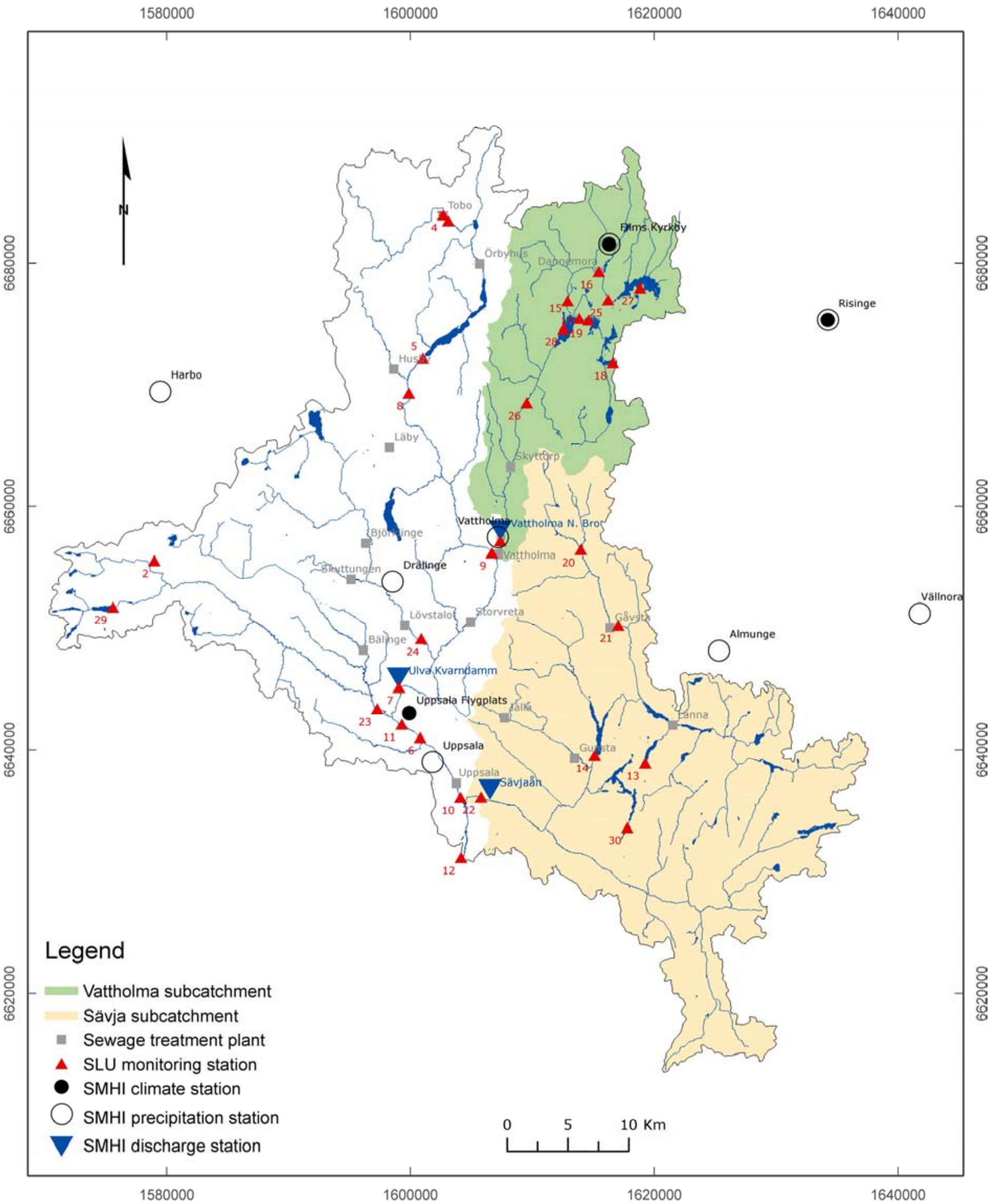

Figure 5.1: Instrumentation network and water treatment plant locations in the Fyrisån catchment.

5.3. Chemistry data

5.3.1. Non-point source emissions

Leaching coefficients

As pointed out in the preceding modelling section, terrestrial leakage was considered within the model approach by using the standard nitrogen leaching coefficients that were associated with different land use types within the research area. Due to the important role of diffuse nitrogen pollution from agricultural land as one of the major sources of nitrogen load to groundwater and surface waters (e.g. STALNACKE et al. 1999; KYLLMAR 2004), special emphasis was given to a detailed derivation of spatial heterogeneity of leaching from arable land, whereas a simpler homogeneous distribution of leaching was assumed for the remaining land use classes.

Leaching coefficients for arable land were obtained from the TRK project (BRANDT et al. 2002; JOHNSSON et al. 2002) and have been calculated by the SOILNDB model (cf. 4.3.3) for 13 different crop groups and 10 soil texture classes for 22 production-climate regions in Sweden. These were assumed to be relatively homogeneous with respect to climate and farming. In this study, outputs from the SOILNDB model for leaching region six of the TRK project were chosen, as they were representative for the Fyrisån region. Table 5.2 gives an overview of the obtained values depending on crop group and soil class.

Table 5.2: TRK leakage coefficients.

	Sand (mg l^{-1})	Loamy sand (mg l^{-1})	Sandy loam (mg l^{-1})	Loam (mg l^{-1})	Silt loam (mg l^{-1})	Sandy clay loam (mg l^{-1})	Clay loam (mg l^{-1})	Silty clay loam (mg l^{-1})	Silty clay (mg l^{-1})	Clay (mg l^{-1})
Area (%)	0	0	4	11	3	1	27	9	14	31
Spring barley	12.2	11.6	10.7	10.5	10.2	9.0	7.9	7.1	5.4	4.6
Winter wheat	10.7	10.6	10.2	9.9	9.8	8.4	7.9	7.1	5.2	4.2
Ley	6.3	4.9	2.6	2.1	1.5	2.0	1.3	1.1	1.0	0.9
Green fallow	10.3	9.2	5.7	4.4	3.6	4.0	2.7	2.3	1.8	1.6
Oats	11.6	11.1	10.6	10.7	10.5	9.0	8.1	7.3	5.6	4.8
Spring wheat	11.4	10.1	10.0	10.1	10.4	8.5	7.8	7.0	5.4	4.5
Spring rape	13	11.9	10.6	10.2	9.8	8.7	7.5	6.7	5.1	4.3
Pasture			1.0	0.7	0.6	0.8	0.5	0.4	0.4	0.4
Undefined arable land			7.2	6.8	6.4	5.9	5.0	4.5	3.4	2.9
Minor crops			10.5	10.4	10.2	8.9	7.9	7.1	5.4	4.6

In order to achieve a thorough spatial description of nitrogen leakage from arable land, the respective leakage coefficients were combined with all available information of underlying soil, land use distribution, crop growth, and agricultural field location. Therefore detailed data of the year 1999 on crop distribution was obtained from the IAKS (Integrated Administrative Control System) data base that is based on applications for EU agricultural subsidies. Geographic boundaries of the agricultural parcels were derived from the block data base of the Swedish Board of Agriculture for the years 1999 and 2000. In addition a soil map for whole Sweden based on 3100 samples differentiating 12 soil types according to the international soil type classification system was available (ERIKSSON et al. 1999).
The subsequent spatial delineation approach followed a step-wise procedure. In a first step, spatial data on field and soil distribution were linked resulting in a data base with information on more than 11 000 field parcels and their respective crop and soil class in the Fyrisån basin. In a second step, the leaching coefficients obtained from the TRK project were associated with the respective soil and crop classes of the obtained data base. Areas with missing information were assigned mean leakage coefficients by interpolation from neighbouring grid cells. In a last step the obtained leakage coefficients were resampled to the model resolution of 250 × 250 m², whereby they were scaled by the sub-grid distribution of arable land in order to achieve an area accurate description by the model. The result was the most detailed spatial description of leaching from arable land within the Fyrisån drainage basin. Other studies on nutrient transportation in Sweden frequently used the same kind of data sources (e.g. ANDERSSON et al. 2005), but most of the spatial heterogeneity that can be assessed by a distributed model was neglected in studies which employ lumped or semi-distributed model approaches.

Nitrogen leakage from forest is normally very low and much smaller than atmospheric deposition, as most intact forest ecosystems tend to retain nitrogen. Different studies on leakage from forest ecosystems have been carried out in Sweden, but mostly in headwater catchments and at small scales and with varying results. Due to great heterogeneity in underlying soil types and deforestation status it is difficult to derive spatial variable leaching coefficients. This situation applies also to the other land use classes wetland and settlement, since arable land is by far the largest contributor to nitrogen load in the Fyrisån and no further detailed spatial information about other land use classes were available. This is why it was considered as sufficient to apply homogeneous leaching factors for these land use classes as it is frequently seen in other model applications (Table 5.3).

Table 5.3: Constant leaching coefficients for forest, wetland and settlement (from TJERNELL 2005).

Land use	Leakage (kg/ha)	Leakage (mg/l)	Source
Forest	1.02	0.60	KYLLMAR (1995)
Wetland	2.04	1.20	SONESTEN et al. (2004)
Settlement	2.00	1.18	BEXELIUS (1999)

Atmospheric deposition

Dry and wet atmospheric deposition of nitrogen was obtained from the MATCH (Mesoscale Atmospheric and Chemistry) model (LANGNER et al. 1995). MATCH is an atmospheric dispersion model including physical and chemical processes governing sources, atmospheric transport, and sinks of oxidised sulphur and oxidised and reduced nitrogen. It has been developed as a tool for mapping of air pollution deposition and concentration over Sweden and for air pollution assessment studies. Yearly raster data covering whole Sweden with a resolution of 20×20 km² was available and downloaded for the application period of the study for the time period 1992 to 2004 (MATCH 2005). For the missing year 2005 in the MATCH outputs a yearly mean deposition map computed from preceding years was used.

Due to the coarse grid resolution, the raster data was interpolated to a 250×250 m² resolution utilising inverse distance weighting between the mid points of the coarse grid cells that were covering the Fyrisån drainage basin. The data was further adjusted to a daily time step and included as nitrogen deposition on open water courses and lakes in the model simulation. Nitrogen deposition on other land use forms is inherently considered by the leaching coefficients derived by the SOILNDB model (cf. 4.3.3).

5.3.2. Point source emissions

Waster water treatment plants

Punctual discharges from municipal water treatment plants were available for several stations throughout the drainage basin (cf. Appendix). Detailed discharge and analytic chemical records were provided from the commune of Uppsala (Uppsala komun) with a temporal resolution of control samplings ranging from daily to monthly applications. Statistical analysis and visual inspection revealed a heterogeneous and highly variable character of the data sets and no further trend or consistent correlation to meteorological and hydrological driving variables could be identified. Hence a simple linear interpolation approach was chosen to obtain daily stream inputs as required by the model.

Rural households

In the recent discussion on eutrophication of surface water bodies in Sweden diffuse emissions from private sewages or so-called rural household emissions are assumed to play a key role in contributing considerably to river pollution (e.g. ARHEIMER et al. 2005). Applications of nutrient transport models would be one measure to assess possible impacts on river pollution, but are unfortunately mostly constrained by the lack of detailed input data such as location of houses, number of inhabitants, and the employed sewage system. One further emphasis in the preparation of input data was therefore the compilation of data concerning rural households in the research area in order to assess possible impacts on water quality. This was achieved in cooperation with the county administration (Länsstyrelsen) which prepared and provided available data from the municipalities within the Fyrisån catchment. Altogether data sets from more than 10 000 cadastral parcels were obtained. Besides the location of each parcel, for most data sets also the number of inhabitants and the type of residence was specified, whereas information on the type of domestic sewage treatment was available only for some data sets.

To consider all available information on sewage treatment, but to also include data sets with missing information, a scenarios was elaborated that accounted for all rural households within the region and is based on assumptions and procedures adopted from prior studies (TJERNELL 2005).

For the population regarded as a diffuse emitter, a specific load of total 5050 g N a^{-1} $person^{-1}$ was considered as recommended by VINNERÅS (2002). This value was corrected by a factor of 0.7 according to FALCK (1996) to account for average presence of the person per year. Further assumptions were 2.5 persons on average per household and a frequency of utilisation of summerhouses from two month (July, August) per year (EKSTRAND et al. 2003; KVARNÄS 1996). Data sets with no specific information on the kind of residence (permanent or summer house) were distributed randomly according to statistics obtained form EHJED & MALANDER (2004). Normally a retention factor of 0.74 is assumed (EHJED & MALANDER 2004) for rural household emissions to account for available measures to reduce nitrogen source emissions, such as a sand filter. In this study no retention was assumed in order to simulate a worst case situation for the rural households in the catchment.

5.3.3. Water chemistry monitoring network

Water chemistry parameters were obtained from a routine monitoring programme of the Department of environmental assessment of the SLU (Institutionen för Miljöanalys). The routine monitoring included a wide range of chemical parameters varying from nutrient fractions to heavy metals. Monitoring was achieved in a monthly, sometimes biweekly time step and involved major tributaries and lakes within the Fyrisån catchment (Figure 5.1).

5.4. The Fyrisån data base

The aforementioned preparation of input data for the model application was concluded by the compilation of a central data base including all temporal data that was part of the actual research. Furthermore additional data that was not used during the application period, such as discontinued discharge stations or precipitation and climate records were processed and incorporated. Thus the data base comprehends the current state of the art of available data for hydrological and nutrient transport models in the mesoscale Fyrisån basin and constitutes a valuable data source for further research work. Figure 5.2 gives a synopsis of the structure and data content.

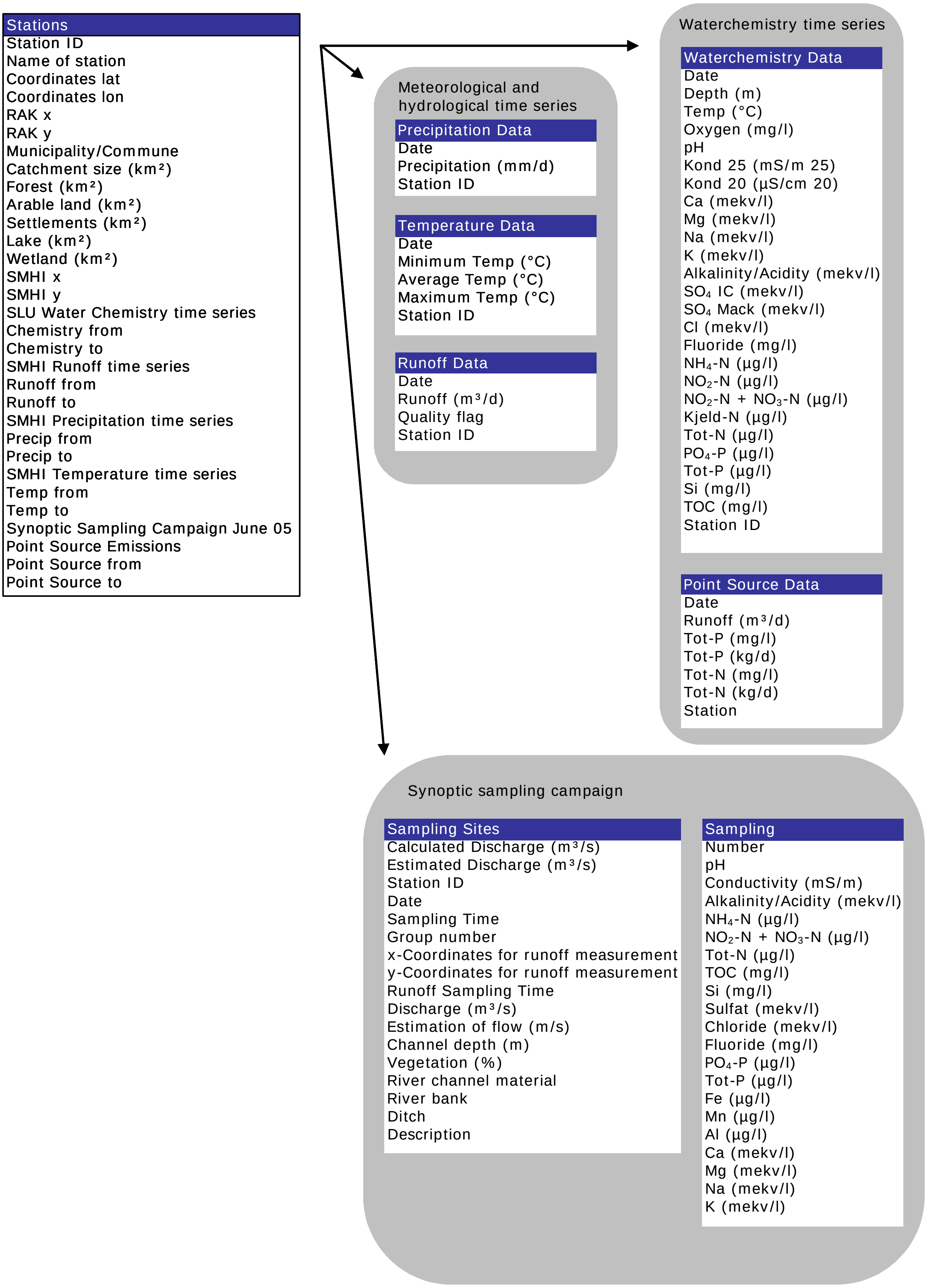

Figure 5.2: Structure and content of the Fyrisån data base.

6. Synoptic sampling campaign

6.1. Basic concept

According to the International Organisation for Standardisation (ISO) water quality monitoring is defined as the process of sampling, measurement and subsequent recording of various water quality characteristics (BARTRAM et al. 1996).

Types of water quality information required by hydrologists include information on background quality as well as temporal and spatial trends in physical, chemical, and biological properties of the aquatic ecosystem. The most important outcome of monitoring programmes is the identification of key causes of poor water quality in a system and allows resources to be directed towards critical problem areas. In general catchment-scale water quality monitoring programmes can be subdivided into three categories (e.g. EYRE & PEPPERELL 1999):

- Routine monitoring
- Event monitoring
- Synoptic or snapshot sampling

Routine monitoring contains periodic collection of sample from a distinct small number of fixed locations throughout the watershed. This approach is mostly ongoing and costly and although water quality problems can be identified, due to low sample density it is mostly problematic to pinpoint the exact causes. In the Fyrisån catchment monthly records of water quality sampling were available from the SLU monitoring programme.

Event monitoring is a flow weighted collection of water quality samples at sample sites typically located at the catchment outlet. It has the advantage that by combining concentration and discharge measurements information about the amount of transported solute can be obtained. Nevertheless this approach also does not identify causes of poor water quality, as effects of point and non-point source pollution occur throughout the catchment and are integrated and diluted.

Thus effective catchment management requires an additional methodology to identify major pollution sources and in-stream processes. This is achieved by a so-called synoptic or snapshot sampling and involves the collection of water from a large number of sample points over a short period of time (GRAYSON et al. 1997). Since most water quality parameters vary with discharge, especially during passage of flood peak, sampling during that time would contain a varying discharge related component. For this reason low flow conditions provide the best opportunity by ensuring stable flow conditions throughout the drainage basin. During stable conditions discharge measurements are essential in addition to water sampling in order to make load calculations for every sample site and to derive concentration values of important chemical parameters. These can be then used to establish load balances or serve as input to solute transport modelling. From the perspective of water quality a further advantage of sampling during low flow recession is based on the fact that low flow periods constitute mostly the critical time for the ecological health of aquatic systems (e.g. MULHOLLAND 1992).

In general this approach provides a detailed picture of the spatial distribution across the catchment and can be used to asses the influence of geology, soil, land use, in-stream processes, and point sources on water quality (GRAYSON et al. 1997). In spite of this apparent utility of the approach not many applications were reported yet, but an increasing number of recent studies that employ this sampling approach, indicates its rising popularity. (EYRE & PEPPERELL 1999; GRAYSON et al. 1997; SALVIA et al. 1999; TOURNOUD et al. 2005; WAYLAND et al. 2003).

In the course of this study a synoptic sampling campaign was planned and carried out in the Fyrisån catchment which objective was twofold: On the one hand the applicability of the method of spatially intensive water quality monitoring should be assessed with regard to further applications, while on the other hand the obtained hydrologic and chemistry data should be used to evaluate both the hydrological as well as the coupled nutrient transport model with respect to spatially variable runoff and nutrient patterns. To achieve this task, stream sampling in combination with current meter measurements were performed. Beyond the scope of this work was a detailed spatial and statistical analysis of the obtained data as demonstrated for instance by WAYLAND ET AL. (2003) and EYRE & PEPPPERELL (1999).

6.2. Experimental details

6.2.1. Rational for the location of sample sites

Different information was assessed and combined to derive the location of sample points within the Fyrisån basin. The data contained: topographical maps, information on land use, vector data of the stream network and lakes, vector data of sub-catchments derived by SMHI and information about the location of point sources of municipal water treatment plants that was obtained from the commune of Uppsala.

The locations of the sample sites were selected according to following, sometimes competing criteria:

- Sample sites ensure a longitudinal profile of water quality along the Fyrisån and its tributaries, accounting for most tributary junctions.
- Upstream and downstream sampling from lakes and point source input (municipal water treatment plants).
- Sample site locations similar to location of monthly monitoring sites of SLU.
- Accounting for sub-catchment arrangement along the stream.
- Evenly spaced sample sites.
- Ease of access to the sample sites, located at bridges or other easily accessible locations to speed up the sample process.

As a result from this decision process 100 sample sites for the sampling campaign were identified. Some samples were taken in duplet or triplicate to assess analytical error and variation during stream flow. For one third of the points additional stream flow measurements were intended to complete stream flow data from the three main runoff stations throughout the catchment in order to enable load calculations (Figure 6.1).

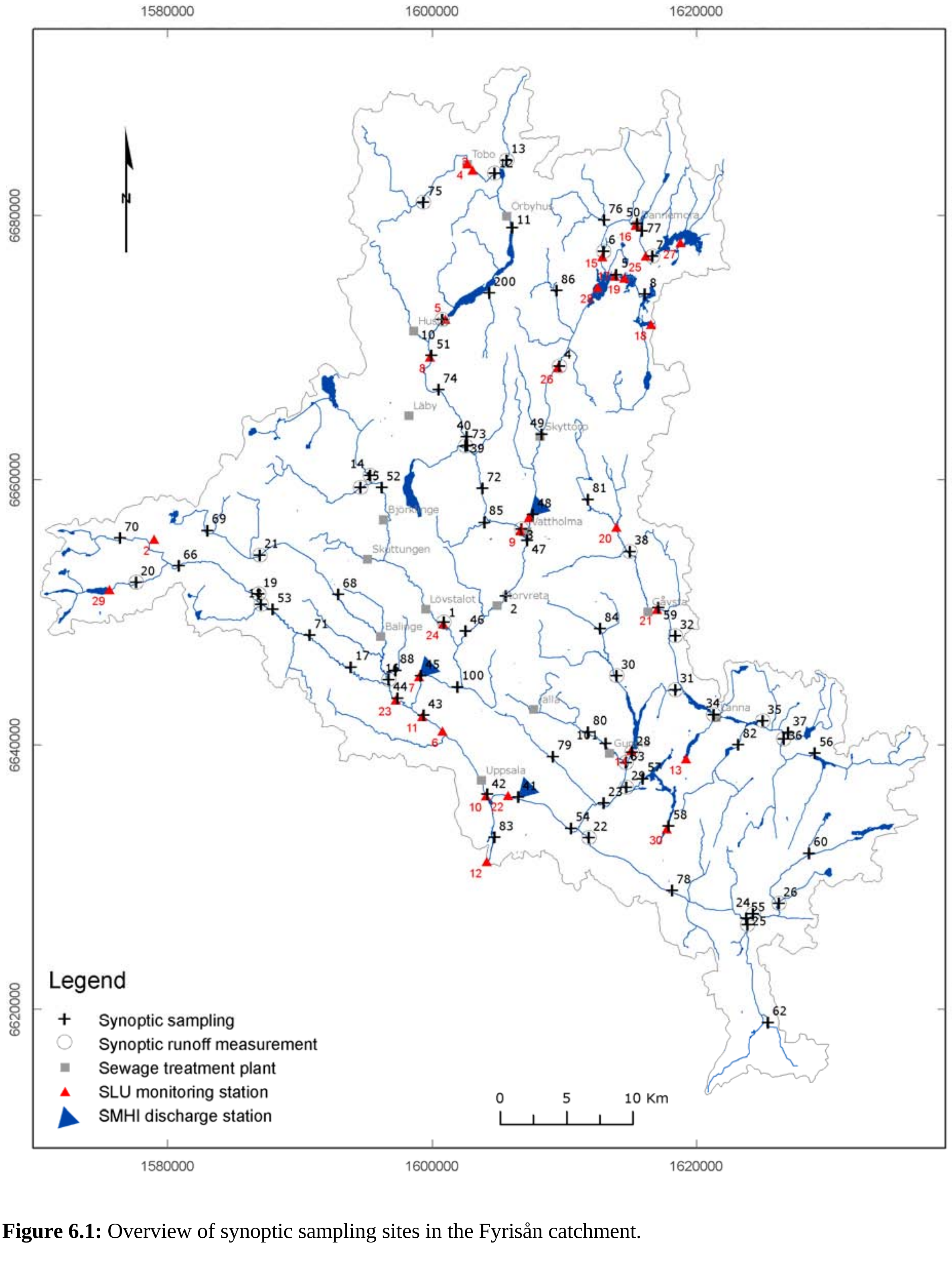

Figure 6.1: Overview of synoptic sampling sites in the Fyrisån catchment.

6.2.2. Sampling

Synoptic sampling was conducted over a two day period from the 28th to 29th of June 2005. The fundamental prerequisite for the initialisation of the snapshot sampling campaign are stable flow conditions which were present during this period, since the hydrograph was in the later stages of the recession limb and discharge remained nearly constant during the sampling period.

Sampling was carried out during both days by six teams of two or three people. These teams were simultaneously collecting at different locations throughout the catchment. Each group was equipped with a sampling kit, containing sample location maps, GPS and sample bottles. Additionally four groups were equipped with current meters to measure discharge at selected sample sites. Training was provided to each group at the first sample point to standardise sampling and measurement procedures.

According to these procedures samples were taken at each site from the thalweg of the river approximately 10 cm below the water surface, being careful not to disturb the bottom or to include surface scum in the sample. Sampling was done with plastic bottles or a bucket from bridges that were rinsed three times with water before the sample was taken.

At selected sites, additional stream flow measurements were conducted with OTT and SMHI current meters choosing a limited number of measurement verticals and points in order to ensure a quick sample and measurement propagation during the sampling campaign. Thus a reduced two-point method was applied for current meter measurements following standard hydrometric procedures by HERSCHY (1999) and USGS (2005). If the water depth was more than 60 centimetres at the sample site, water velocity was measured at points 0.2 and 0.8 of the depth from the surface, while for smaller depth the 0.6 point depth from the surface was measured. Spacing and number of measurement verticals depended on channel width and are given in Table 6.1.

Table 6.1: Number of verticals used during synoptic stream flow measurements (from HERSCHY 1999).

Channel width (m)	Number of verticals
0 – 0.5	3 – 4
0.5 – 1.0	4 – 5
1.0 – 3	5 – 8
3 – 5	8 – 10
5 – 10	10 – 20
> 10	> 20

Stream flow at remaining sites was estimated according to a simple drift method recommended by SMHI & NATURVÅRDSVERKET (1979). In the course of the campaign altogether 88 sites have been sampled from which about one third contained additional runoff measurements, since some streams were not accessible or dry.

Figure 6.2: Synoptic sampling and discharge measurements at different sites in the Fyrisån catchment.

6.2.3. Laboratory analysis

The collected samples were stored cold and nutrient parameters were analysed within a few days. Analyses were conducted by the laboratory of the Department of Environmental Assessment at SLU. Samples were analysed for following different fractions of nutrients: Total nitrogen (Tot-N), nitrate and nitrite-nitrogen (NO_3+NO_2-N), ammonium-nitrogen (NH_4-N), total phosphorous (Tot-P) and phosphate (PO_4-P). In addition samples were also analysed for following chemical parameters: total organic carbon (TOC), Sulphate, Chloride, Fluoride, Si, Fe, Mn, Al, Ca, Mg, Na, K, pH, Conductivity and Alkalinity/Acidity. Applied analytical methods including measurement ranges and analytical errors can be found in the Appendix. In the course of this study only nitrogen species will be subject to further analysis, while other parameters were beyond the scope of this thesis.

6.2.4. Calculation of runoff and loads

A current-meter measurement is defined as the summation of the products of the subsection areas of the stream cross section and their respective average velocities (USGS 2005):

$$Q = \sum (a \cdot u) \qquad \textbf{Eq. 5.1}$$

Q: Total discharge ($m^3\,s^{-1}$)
a: Individual subsection area (m^2)
u: Mean velocity of flow normal to the subsection ($m\,s^{-1}$)

For the computation of discharge data a midsection method of computing a current-meter measurement was applied (USGS 2005). It assumes that the velocity sample at each vertical represents the mean velocity in a rectangular subsection. The subsection area extends laterally from half the distance from the preceding observation vertical to half the distance to the next, and vertically from the water surface to the sounded depth.

The cross section is defined by depths at the verticals. At each vertical the velocities was sampled by current meter to obtain the mean velocity for each subsection. As different types (SMHI and OTT) of current meters were used during the campaign, different kinds of raw data was obtained. While some devices provided the mean velocity values directly for each measurement point in a vertical based on internal conversion of propeller rotation to stream velocity, others gave only the number of propeller rotation per discrete time interval. In the latter case the mean velocity was derived based on a respective calibrated conversion function for each current meter. The subsection discharge was then computed for any subsection at vertical x by use of the equation:

$$q_x = v_x \cdot \left(\frac{(b_x - b_{(x-1)})}{2} + \frac{(b_{(x+1)} - b_x)}{2} \right) \cdot d_x = v_x \cdot \left(\frac{(b_{(x+1)} - b_{(x-1)})}{2} \right) \cdot d_x \qquad \textbf{Eq. 5.2}$$

v_x: Mean velocity at vertical *x* (m s^{-1})
b_x: Distance from initial point to vertical *x* (m)
$b_{(x-1)}$: Distance from initial point to preceding vertical (m)
$b_{(x+1)}$: Distance from initial point to next vertical (m)
d_x: Depth of water at vertical *x* (m)

The summation of discharges for all subsections results in the total discharge of the stream. Besides the current meter measurements, stream flow estimations based on the drift method were used to derive discharge estimates. Since drift measurements reflect mainly the stream velocity at the water surface, an empiric correction factor based on channel characteristics was applied according to SMHI & Naturvårdsverket (1979):

$$Q = k \cdot v_{\max} \cdot A_{mean} \qquad \textbf{Eq. 5.3}$$

Q: Discharge (m s^{-1})
k: Correction factor (-)
v_{max}: Measured velocity of surface stream flow (m s^{-1})
A_{mean}: Mean average cross sectional area of measuring section (m^2)

Table 6.2: Empirical k-parameter for the correction of stream flow estimates.

k value			
rough channel, stones, reed and grass	channel stones	planar channel, sand or gravel	planar, artificial stream section
0.5	0.6	0.7	0.8

In general the drift method suffered from a large uncertainty resulting in a large scatter of the obtained values. By applying the empirical correction factor depending on the stream section characteristics of each sample site, this scatter could be reduced significantly, but still large uncertainties remain in comparison to the current meter derived values. A measurement error of ± 10 % was assumed for the current meter measurements for further application in this study, while flow estimates contain a substantially higher error.

Based on this computation instantaneous fluxes at every station were calculated by multiplying the obtained instantaneous concentrations with the calculated corresponding discharge. Specific fluxes were obtained by dividing the derived instantaneous fluxes by the upstream area of the sourceshed at each station.

6.2.5. Sourcesheds and land use distribution

Sampling points and land use distribution were related by the development of surface water sourcesheds derived from a 90 × 90 m² SRTM DEM (cf. 5.1.1). A sourceshed is defined as the total area that contributes to a selected drainage or sampling point (e.g. WAYLAND et al. 2003). For each sampling point a respective sourceshed was generated and the associated percentage of land use type (forest, agriculture, urban area, wetland, and lake) (cf. 5.1.3) was calculated. The obtained water chemistry data for each sample point was then linked to land use class distributions for the corresponding sourceshed in a central data base. The data base allowed correlations of obtained chemical parameters from each sample site and environmental attributes in terms of land use.

6.2.6. Water quality classification

Water quality was classified according to the national Swedish environmental quality criteria for surface waters and lakes (EPA 2000; LINDBERG 2001). These criteria are normally intended to judge nitrogen concentration by long term averages, but can be also used as an indicator for nitrogen concentrations derived by snapshot sampling. The high sampling density of the snapshot campaign allowed to produce a detailed map of the nitrogen concentration patterns for the sampling period that was colour coded according to the given water quality concentration ranges (Table 6.3).

Table 6.3: Classification of Tot-N concentrations according to the Swedish water quality criteria (from EPA 2000).

Class	Description	Tot-N concentration (mg/l)
1	Very low concentrations	< 0.300
2	Low concentrations	0.300 - 0.450
3	Moderately high concentrations	0.450 - 0.750
4	High concentrations	0.750 - 1.500
5	Very high concentrations	> 1.500

6.3. Results

From a hydrologic standpoint the sampling campaign took place in a quasi steady state condition after the spring flood. Thus the prerequisite of stable flow conditions was achieved during the sampling campaign.

6.3.1. Spatial patterns in water quality and stream flow

Figure 6.3 shows the spatial distribution of Tot-N concentrations in the Fyrisån catchment. The concentration classification according to the Swedish Environmental Quality Criteria (EPA 2000) reveals in general rather high nitrogen concentrations throughout the catchment ranging from 0.36 mg/l to almost 3 mg/l. Starting form headwater streams, a general increase in Tot-N concentrations towards the outlet is noticeable. Exceptions with higher Tot-N concentrations are apparent for some headwater areas in southern part of the Sävja drainage basin and also in northern parts of the Vattholma and Vendelån watersheds, where arable land with intensive farming is the predominant land use form. Unlike the southern Sävjan region, theses areas are characterised mainly by forest, some rural households as well as smaller settlements (Tobo, Örbyhus and Österbybruk) that are connected to central sewage treatment plants contributing with their emissions directly to the stream. Besides these examples, an increase of Tot-N concentration downstream of single treatment plants could be observed frequently throughout the catchment. In contrast to headwater areas that are in general dominated by forest, the central region of the Fyrisån catchment is dominated by intensive farming and reveals consistently higher concentration values. The highest Tot-N concentration values could be observed below the city of Uppsala and in the region around the lakes Trehörningen and Funbosjön that are popular holiday areas close to Uppsala.

6.3.2. Spatial evolution of nutrient concentrations along the Fyrisån

Concentration values were combined with discharge values and enabled the calculation of nitrogen loads along the Fyrisån. Figure 6.4 presents the evolution of Tot-N loads and nitrogen species (NH_4-N, NO_3-N) loads along the river. Moreover the measured fluxes F_i (kg d^{-1}) at every station *i* were compared with the expected fluxes according to a procedure adopted from (SALVIA et al. 1999). The expected fluxes were derived from the sum of measured instantaneous fluxes (F_{i-1}) at the closest upstream station (*i-1*) and incoming fluxes by tributaries between station *i* and *i-1*. This methodology may allow the quantification of additional inputs betweens stations as well as the estimation of potential retention in the river section. Additionally the corresponding concentration profiles are presented (Figure 6.5).

To begin with discharge, a general increase of discharge values from headwater catchments to the outlet in Flottsund could be observed reflecting the increase in catchment size and the several tributary junctions on the way downstream. The spatial evolution of nitrogen loads followed a similar trend. However, differences were noted for single station and nitrogen fractions along the river. Starting from headwaters, sample site 7 is characterised by comparatively low nitrogen concentration values and loads. The main part of the Tot-N concentration and loads at site 7 is dominated by the organic fraction of nitrogen. This situation is also characteristic for the downstream sites up to site 48 (Vattholma) that are mainly forested. From site 48 onwards the Fyrisån runs across more intensively cultivated land and Tot-N is composed essentially of nitrates that constitutes up to 70 % of the Tot-N at some stations. This high fraction of nitrate is constantly increased towards the catchment outlet at Flottsund.

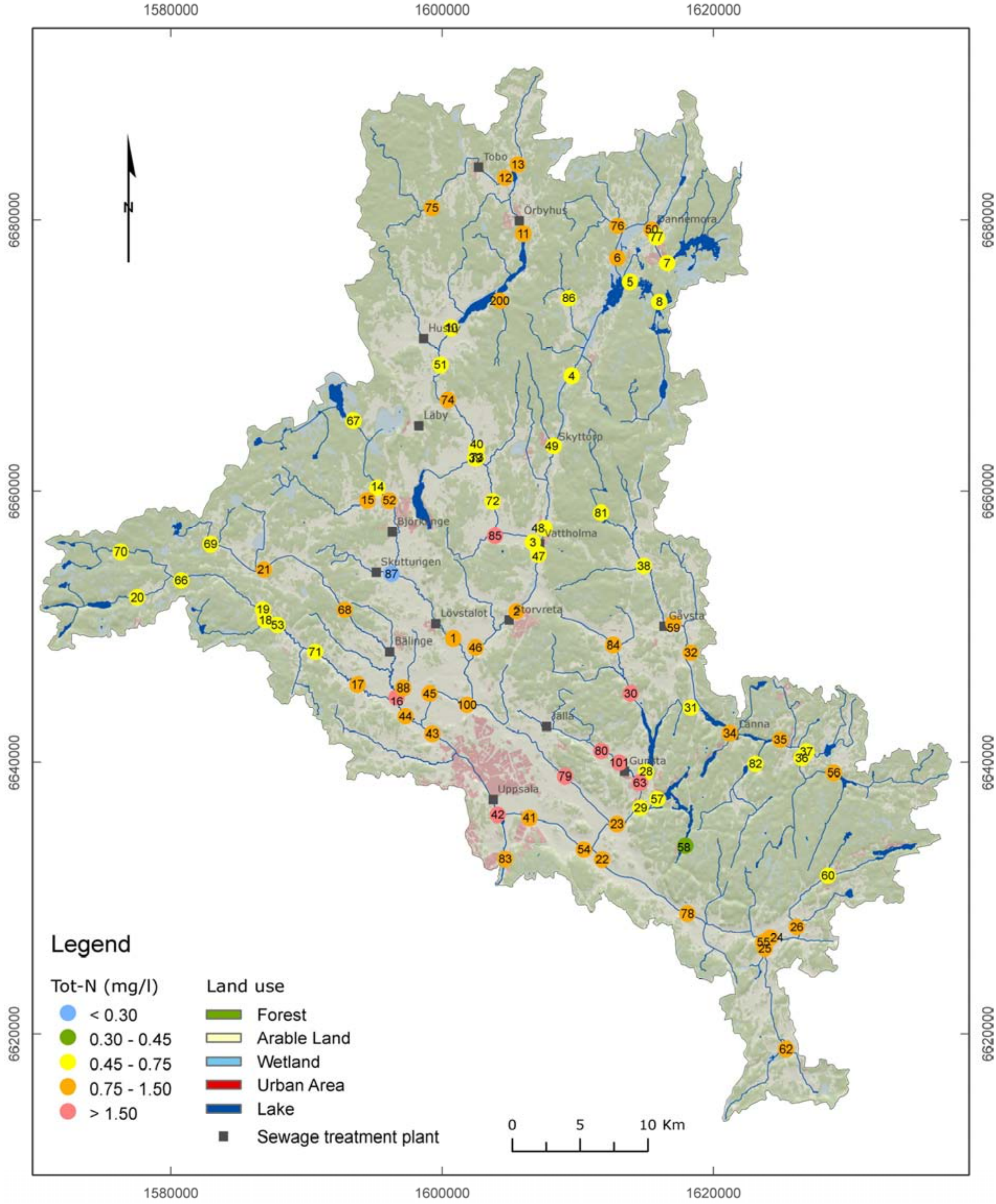

Figure 6.3: Spatial patterns of Tot-N concentrations and classification according to the Swedish environmental water quality criteria.

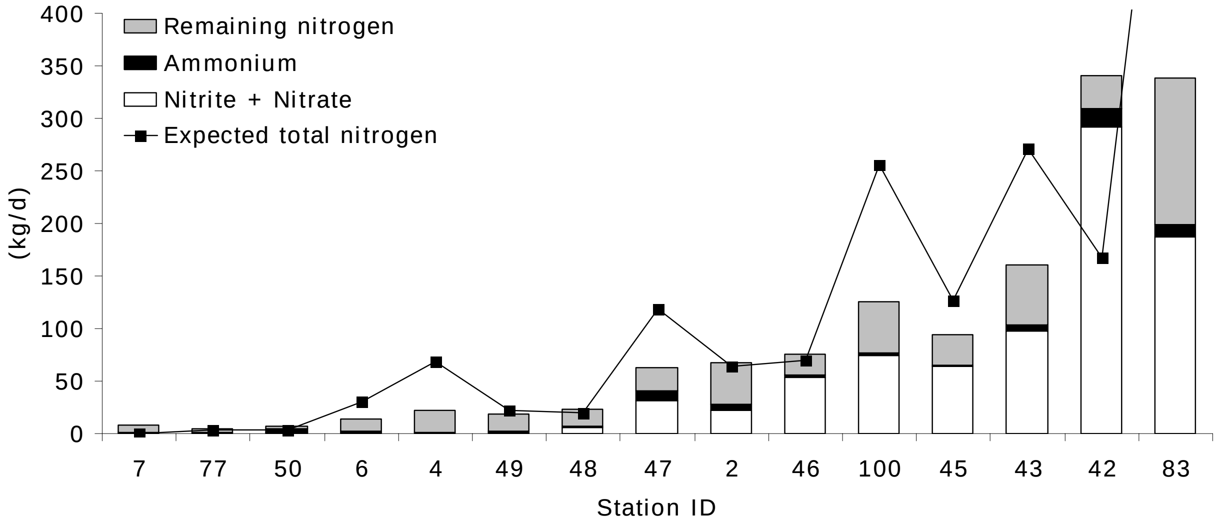

Figure 6.4: Measured and expected synoptic nitrogen loads along the Fyrisån.

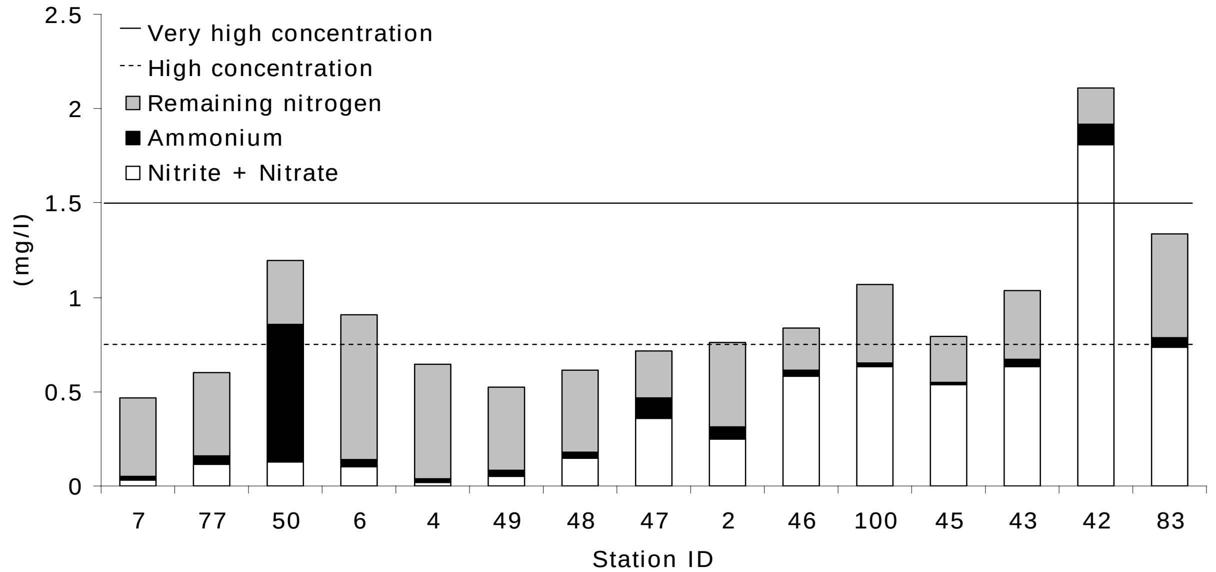

Figure 6.5: Concentration profiles of synoptic nitrogen concentrations along the Fyrisån.

Besides this general trend, ammonium concentrations and loads are relatively low. Significant differences in concentrations can be consistently observed downstream from water treatment plants. A prominent example is sampling site 50 situated directly below the water treatment plant of Dannemora. At this site ammonium is the most dominating nitrogen fraction, while nitrate concentrations are only slightly increased. However, this high increase in concentration is followed by a decrease of ammonium between the sites 50 and 6 down to initial concentrations of nitrogen.

Other sampling sites characterised by water treatment plants emissions are site 46 that is influenced by the Vattholma treatment plant and reveals higher ammonium and nitrate concentrations and site 42 that is located directly downstream of the central water treatment plant of the city of Uppsala. Consequently it shows a massive increase in nitrate concentrations alongside with a comparatively little increase in concentration of the ammonium fraction. An overall decrease of Tot-N concentration could be observed between sample sites 50 and 49 and between sample site 100 and 45, for the latter sample site the nitrogen load was also reduced, while for all other stations nitrogen loads are constantly rising in down stream direction. The graph of the calculated expected nitrogen fluxes peaks five times significantly at the sites 6, 47, 100, 43 and 83 exceeding observed nitrogen loads and therewith indicating the influence of major tributary junctions.

6.3.3. Relation between water quality parameters and environmental attributes

Regression analysis of major land use characteristics (agriculture, forest, urban area, lake and wetland) was carried out with chemical parameters obtained by synoptic sampling (cf. 6.2.5). Significant relations between land use percentage of the respective sourcesheds and nitrogen concentrations could be observed for agriculture, wetlands and lakes.

While Tot-N concentrations are positively correlated to increasing agricultural percentage, a further distinction between different nitrogen fractions reveals the dominating influence of nitrate and nitrite in comparison to the other nitrogen fractions (Figure 6.6). Moreover the relation between Tot-N and wetland and lake percentages shows an oppositional characteristic with decreasing Tot-N concentrations for increasing wetland and lake percentages (Figure 6.7 and Figure 6.8).

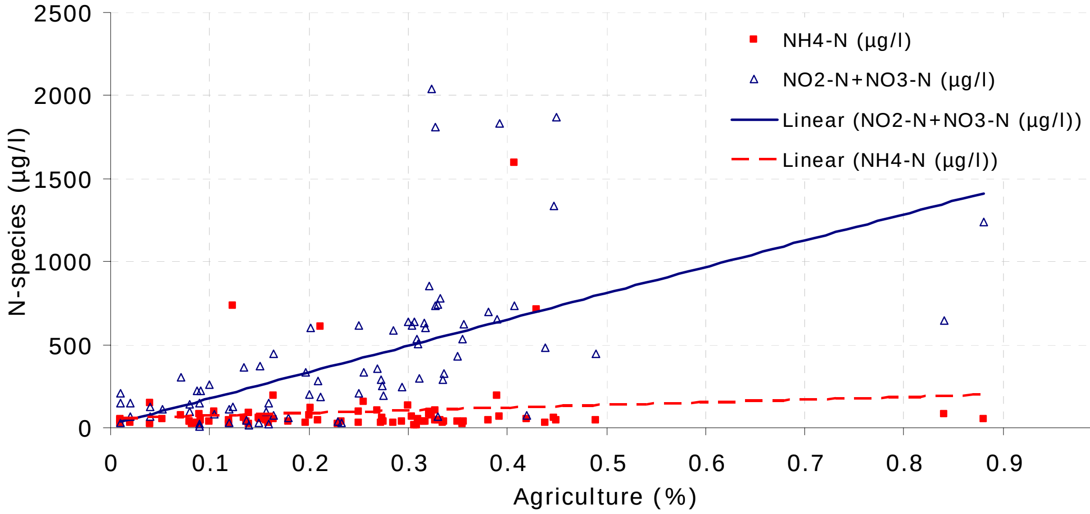

Figure 6.6: Relations between NH_4-N, NO_2+NO_3 and percentage of agriculture for the synoptic sample sites.

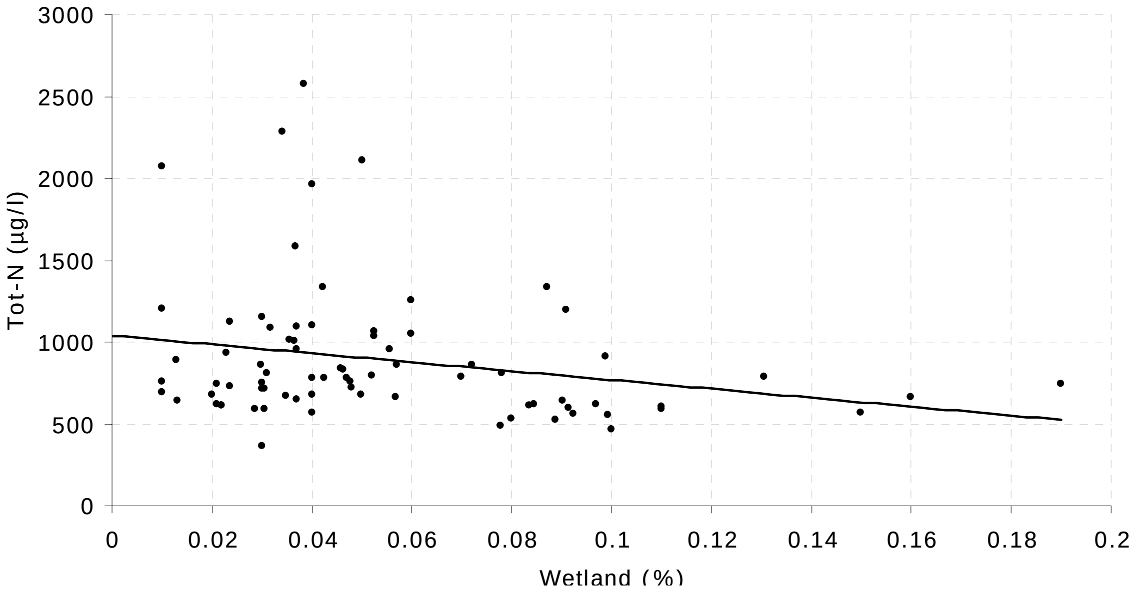

Figure 6.7: Relations between Tot-N and percentage of wetland for the synoptic sample sites.

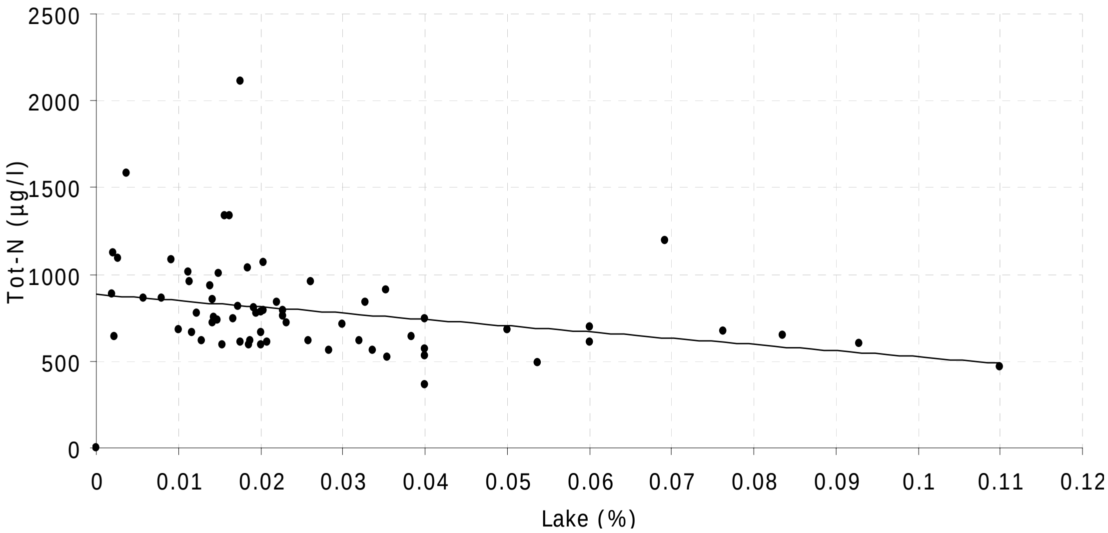

Figure 6.8: Relations between Tot-N and percentage of lake for the synoptic sample sites.

6.4. Discussion

Water quality parameters are typically highly variable spatially and temporally due to various point and non-point emissions and a multitude of chemical, biological, and physical in-stream processes. Besides the variability, measurements of chemical parameters as well as discharges are subject to measurement and analytical errors. Thus associated uncertainties must be considered, when interpreting spatial patterns of chemical parameters or relations to land use or hydrological characteristics. Moreover, it must be considered that the obtained daily fluxes cannot be used to calculate annual loads, due to the large annual variability of hydrologic conditions throughout the catchment leading to a large increase of concentrations during high flow periods.

Nevertheless, in this study significant relations between landscape characteristics and chemical parameters could be identified. The spatial pattern of Tot-N concentration obtained from the synoptic sampling campaign agrees in principal with the findings of the monthly monitoring programme of the SLU (cf. 3.4). These findings imply that arable land constitutes mainly to the nitrogen species nitrate and nitrite in the Fyrisån, since nitrate is easily mobilised from arable land by precipitation and its transportation is favoured by agricultural drainage systems in the region. Hence it may be transported continuously with the river if no losses due to denitrification occur. Figure 6.6 supports these findings with the positive correlation of the NO_2-N and NO_3-N species with increasing percentage agriculture in each sourceshed. This correlation becomes also obvious in Figure 6.4 and Figure 6.5 where high nitrate and nitrate concentrations and loads could be observed for the lower reaches of the Fyrisån that is characterised by intensive farming. In view of Tot-N concentrations, nitrate and nitrite constitutes most to the Tot-N content in those areas. This is also visible in the spatial concentration pattern (Figure 6.3) showing comparatively higher Tot-N concentrations and loads in central areas of the Fyrisån drainage basin, but also in areas in the south of the Sävjåan sub-catchment and in the drainage basin of the River Björklinge. In comparison, forested areas tend to show lower nitrogen concentrations and loads, as the western parts and northern parts of the Fyrisån basin imply.

The ammonium fraction of nitrogen is normally easily exchanged and can be seen as an indicator for point source emissions to the river (e.g. LARSSON et al. 1998). Additionally the increase of Tot-N content down stream of point source emitter was frequently observed and becomes obvious both in the spatial pattern of Tot-N in Figure 6.3 and in-stream concentrations and loads along the stream (Figure 6.5 and Figure 6.4). While at site 50 a relatively high fraction of ammonium was found, other water treatment plants showed considerably lower ammonium concentrations, but these were still significant compared to normal background concentrations found along the stream. Even the largest treatment plant for the city of Uppsala with more than 120000 inhabitants showed besides a doubled nitrate content only a slight increase in ammonium concentration. This can be caused by a variety of factors, but one main influence might be the instantaneous character of the sampling capturing only the characteristic in-stream chemistry at the specific sampling time.

Alongside with this large effect on nitrogen concentration by the city of Uppsala between site 43 and 42 further high nitrogen concentrations are observed particularly in the region around the lakes Trehörnigen and Funbosjön. Besides the two point source emitters Jälla and Gunsta this area is a popular recreation area close to Uppsala and is characterised by the highest density of rural households throughout the Fyrisån watershed utilising private sewer systems. Those partly septic sewer systems are considered as one main contributor to nutrient loads in the region.

The computed expected Tot-N load in Figure 6.4 shows significant peaks for tributary junctions. Although an increase of loads is generally seen at these sites, the expected Tot-N load constantly exceeds the measured nitrogen load indicating potential retention effects along the mainstream. Lakes and wetlands are generally considered to play a key role in nitrogen retention processes (e.g. CARPENTER et al. 1998; GREN 1995). This could be approved by regression analysis for the respective land use types (Figure 6.7 and Figure 6.8). This effect can also be seen both in the spatial concentration pattern of Tot-N upstream and downstream of major lakes (Figure 6.3) and in the concentration profiles along the Fyrisån (Figure 6.5). In particular the point source emission concentrations of Tot-N from the water treatment plant in Dannemora (site 50) are significantly reduced downstream, although an increase of nitrogen load due to tributaries is expected. This may imply retention effects caused by the presence of the Lake Dannemorasjön and surrounding wetlands.

Finally it should be noted that some patterns could not be explained reasonably or should be handled with care. For instance the reduction in loads and concentrations between sites 100 and 45. Also the concentration and load calculations at site 83, where the Fyrisån discharges into Lake Ekoln should be handled with care, since the flow direction of the river is unstable at this site allowing potential backflow from the lake into the Fyrisån.

6.5. Conclusion

Despite the large uncertainties and temporal variability that is involved in the synoptic sampling methodology it gave further insight into the spatial pattern of nutrients, the propagation along the stream, and relationships between stream nutrient levels and specific land use classes under summer flow conditions. Moreover regression analysis showed the influence of key landscape environments on water quality and thus supports the differentiation of key landscape environments (e.g. lakes, wetlands, and groundwaters) within in the model concept. It also helped to identify potential critical areas to pollution and enabled additional model testing against the spatial pattern of nutrient concentrations.

The synoptic sampling methodology is certainly associated with several limitations that should be addressed briefly. Depending on catchment size, logistics and cost can be large due to the number of sampling teams and equipment involved and calls for an intensive preparation and planning of the campaign. Low flow hydrological stability can be achieved mainly only during summer and favours the quantification of point source emissions. In contrast the contribution of diffuse sources is less pronounced under dry conditions that point sources and groundwater inputs would be most likely more diluted during higher flows. Synoptic sampling ignores seasonal variation so that periodic point source discharges may have been missed and obtained concentration values and loads can not be extrapolated to monthly or yearly estimates.

Some limitations could be overcome by sampling several times over the year to test the robustness of water quality patterns to seasonal variations. However, it would become increasingly difficult to meet constant hydrological conditions across the catchment.

Finally it can be noted that synoptic sampling is regarded as a rapid, cost effective (long term), and robust approach that allows the identification of point and diffuse sources on water quality. Future applications of the methodology might employ more sophisticated statistical analysis or involve additional sampling and analysis of N-isotopes to further asses the origin of different nitrogen fractions in critical problem areas in the Fyrisån drainage basin.

7. Modelling results

7.1. Hydrologic model

7.1.1. Model calibration

Calibration of model parameters against runoff was done for the two sub-catchments Vattholma and Sävja with the inclusion of the runoff station Ulva Kvarn for validation purposes. The simulation period in this study ranges from October 1994 to June 2005, preceded by a two year warming-up period starting in October 1992. This period is divided into two sub-periods of five years starting with the calibration period October 1994 to September 1999 and followed by a validation period from October 1999 to June 2005.

The model application started with the initialisation of the hydrologic model. Therefore the model was run with the best known parameter set for the entire application period and the generated model outputs were used to set up the model storages and soil moisture routines to realistic volumes at the beginning of the calibration period. Calibration was achieved against daily runoff measurements at the discharge stations Vattholma and Sävja by employing the automated parameter estimator PEST (cf. 4.1.2). The optimisation by PEST was based on the R_V criterion, computed of measured and simulated runoff time series for the respective runoff stations.

Model validation was conducted step-wise according to the hierarchical scheme for systematic testing of hydrological simulation models proposed by KLEMES (1986). In a first step the model was calibrated for the sub-catchments Vattholma and Sävja individually. Afterwards the best derived parameter set for each catchment was exchanged consecutively and used for a new model simulation in the adjacent catchment following the proxy-basin test procedure. In a second step the model was calibrated simultaneously on both catchments in order to determine an optimal single “common” parameter set and in a last step all so far derived parameter sets underwent a traditional split-sample test by applying them subsequently from the calibration time span to the specified validation period.

7.1.2. Split-sample test

The results of the individual catchment calibration showed satisfactory fits between measured and simulated discharge for the calibration period with R_V values between 0.85 and 0.90. No systematic error between high and low flow was evident throughout the calibration period. However, R_V values were considerably lowered during following validation, but still remained on an acceptable level. Noticeable is a strong decline during the validation period from 0.90 to 0.73 (R_V) for Vattholma compared to 0.85 to 0.77 (R_V) for Sävja. Table 7.1 contains an overview of the simulation results with specific objective functions for each catchment.

A similar model performance could also be observed after multi-scale validation using the individual optimised parameter sets in the respectively other watershed. While the R_V values for the first five year period remained on a still sufficient level of 0.73 and 0.76 the next five years showed significantly poorer statistical measures with the strongest declines for the Vattholma runoff station. In addition to this rather dramatic decrease of efficiency for the second half of the time period the relative volume error was increased and revealed alongside with the efficiency a systematic underestimation of the flow dynamic and volume by the model. These apparent errors of the model simulation became evident for single years 1996 and 1997 of the calibration period, but were also dominating throughout the second half of the Vattholma runoff record, especially in 2000 and 2004, where years with multiple spring melt peaks prevailed. Figure 7.2 exemplifies the lack of the model to capture the variable runoff situation for this period with almost opposite simulations of the flow dynamic. In contrast, the prevailing model performances are satisfactory and illustrated for the example year 1998 in Figure 7.1. In this case the model is able to capture accurately the entire runoff dynamic on the basis of the individual Vattholma parameter set.

Table 7.1: Overview of statistical performance measures for split-sample and proxy-basin test results.

Catchment used for calibration	Objective function	Vattholma		Sävja		Ulva Kvarn
		1994-1999	1999-2005	1994-1999	1999-2005	1994-1999
Vattholma	R_V	**0.90**	0.73	0.73	0.63	0.79
	R_{eff}	**0.90**	0.73	0.75	0.65	0.81
	V_E	**0.00**	0.03	0.17	0.16	0.18
Sävja	R_V	0.76	0.54	**0.85**	0.77	0.83
	R_{eff}	0.78	0.57	**0.85**	0.78	0.83
	V_E	0.19	0.25	**0.02**	0.06	0.01
Vattholma & Sävja	R_V	**0.83**	0.63	**0.83**	0.77	0.82
	R_{eff}	**0.84**	0.64	**0.84**	0.78	0.83
	V_E	**0.09**	0.13	**0.10**	0.07	0.11

0.00 data included in calibration (01.10.94 - 30.09.99); 0.00 validation (01.10.99 - 30.06.05)

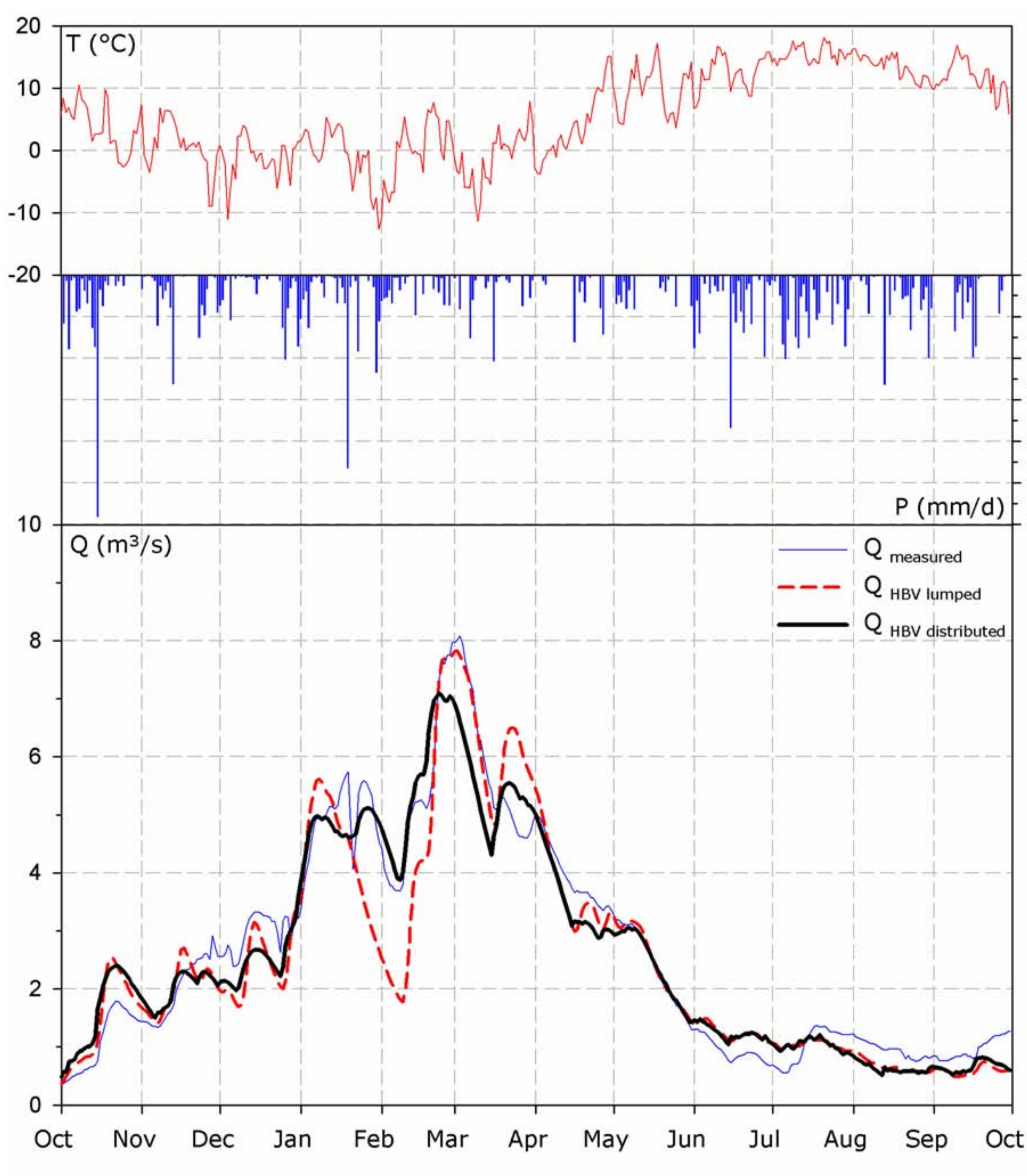

Figure 7.1: Hydrological year with best model fit (1998).

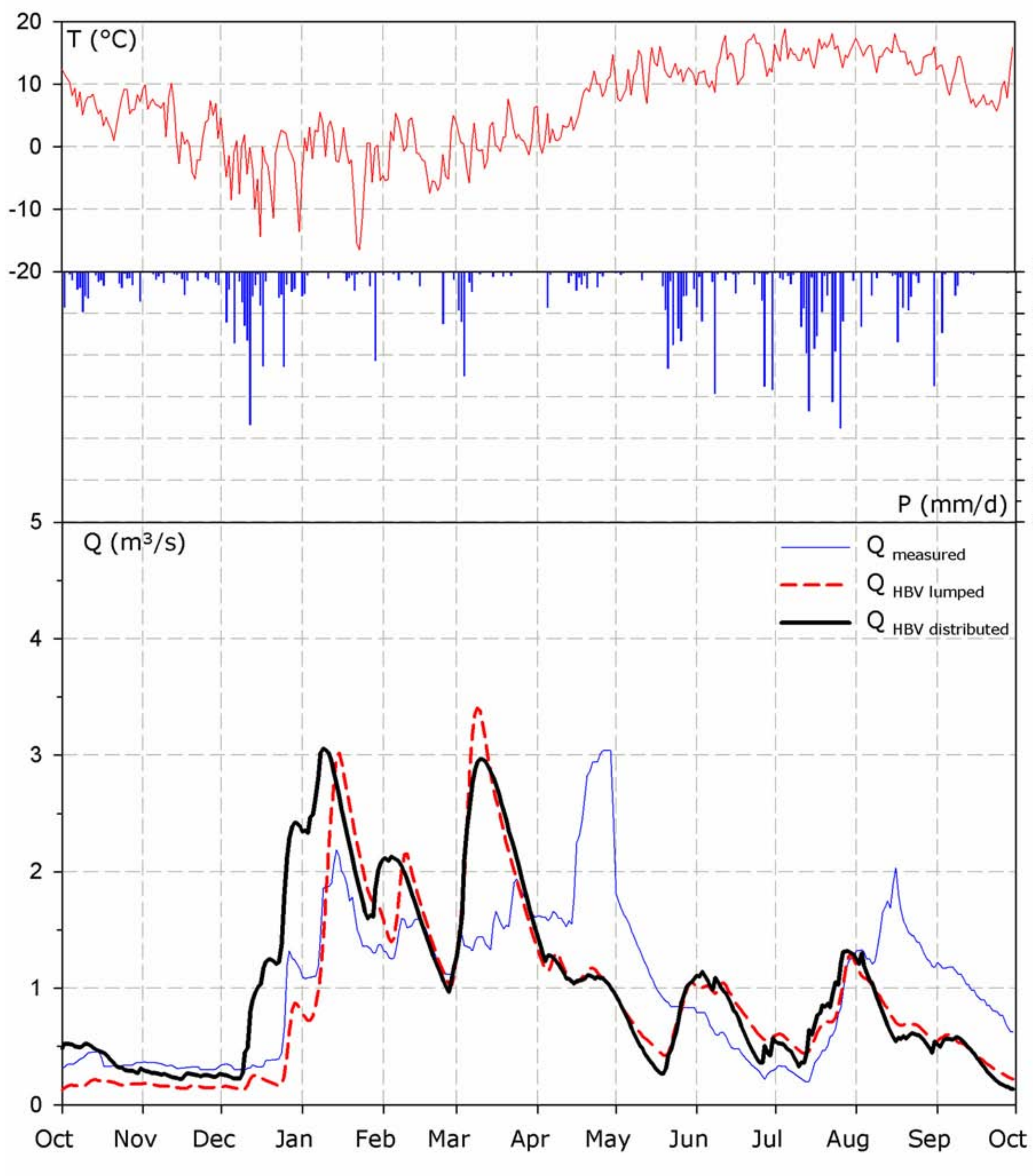

Figure 7.2: Hydrological year with worst model fit (2000).

7.1.3. *Proxy-basin test*

It is interesting to further evaluate the differences between the catchments. Therefore model efficiencies were computed for both sub-catchments using simulated specific discharge of the respective other catchments and the transferred measured specific discharge as it was proposed by SEIBERT ET AL. (2000). Results are listed in Table 7.2 and revealed greater similarities (higher R_{eff}) between the model generated time series than between the measured specific discharges (lower R_{eff}). It is also apparent that the model performed better than transferring the specific discharge between the two catchments.

Table 7.2: Comparison of efficiencies (R_{eff}) derived from different records from Vattholma and Sävja.

Calculation of efficiency between Vattholma and Sävja based on…	Resulting efficiency (R_{eff})[a]
…specific runoff records	0.63
…specific runoff records of Sävja scaled by Vattholma catchment size and compared to Vatthoma runoff records	0.63
…runoff simulations in both catchments	0.84

[a] NASH & SUTCLIFFE (1970)

The aspect of model parameter dependency on individual catchments was further tested with a simultaneous calibration on both catchments to derive a “common” parameter set. This led to a decrease of model performance for the calibration phase compared to the results obtained by individual calibration, but provided an increase of the overall model performance for the whole application period. Validation also included the runoff station Ulva Kvarn with independent runoff records of the calibration phase. In accordance with the preliminary results a best fit could be achieved by the “common” parameter set, therewith representing the optimal parameter set that could be derived in this study for a model application covering the whole Fyrisån basin.

7.1.4. *Model comparison*

To asses the distributed model performance in comparison with a simple lumped model approach, the distributed model outputs were compared to HBV light model results (SEIBERT 2002) using the same regionalised input data (precipitation, temperature and monthly evapotranspiration estimates) for both model applications. Thereby automatic calibration of the HBV light model was achieved by a genetic algorithm (SEIBERT et al. 2000). Based on this best derived “common” parameter set the model intercomparison was carried out subsequently. As illustrated by Table 7.3 it is remarkably that the distributed, highly parameterised model was not able to outperform the simpler, less parameterised HBV model in terms of runoff related efficiency measures. For most years similar model behaviour could be observed resulting for instance in model errors for the same years throughout all catchments which becomes also evident in Figure 7.1 and Figure 7.2. With regard to the overall model performance it has to be stated that the lumped HBV model results are equally well, in some years even slightly superior to the distributed model outputs.

Table 7.3: Comparison of distributed with lumped model results obtained with the "common" parameter set.

Objective function	Vattholma				Sävja				Ulva Kvarn	
	1994-1999		1999-2005		1994-1999		1999-2005		1994-1999	
R_V	**0.83**	0.86	**0.63**	0.74	**0.84**	0.86	**0.78**	0.79	**0.82**	0.84
R_{eff}	**0.84**	0.86	**0.64**	0.76	**0.84**	0.86	**0.78**	0.79	**0.83**	0.84
V_E	**0.09**	0.04	**0.13**	0.01	**0.10**	0.04	**0.07**	0.01	**0.11**	0.05

0.00 results from distributed model; 0.00 results from lumped model

7.1.5. Synoptic runoff measurements

Synoptic runoff measurements provide a further basis for additional model testing by considering spatial variability of river runoff at specific test dates. In connection with a distributed model it is then possible to establish virtual discharge stations within the model simulation to compare its results with runoff measurements along the stream network. Figure 7.3 and Figure 7.4 show a comparison of the measured and simulated river runoff for 22 test sites throughout the drainage basin. In general a sufficient representation of the flow pattern by the model in Figure 7.3 is visible, if one keeps in mind that the measurements represent a snapshot more than five years after the calibration period. Thus the model seems capable to capture the flow generation caused by catchment size in a spatially explicit way as illustrated by the rather well correlation. However, if the influence of catchment size is removed by plotting the specific discharge (Figure 7.4), this correlation is lost indicating that the model has problems to reproduce the spatially induced runoff situation. Subsequent calibration of the model on the synoptic measurements reduced the scatter significantly, but still did not improve the situation sufficiently.

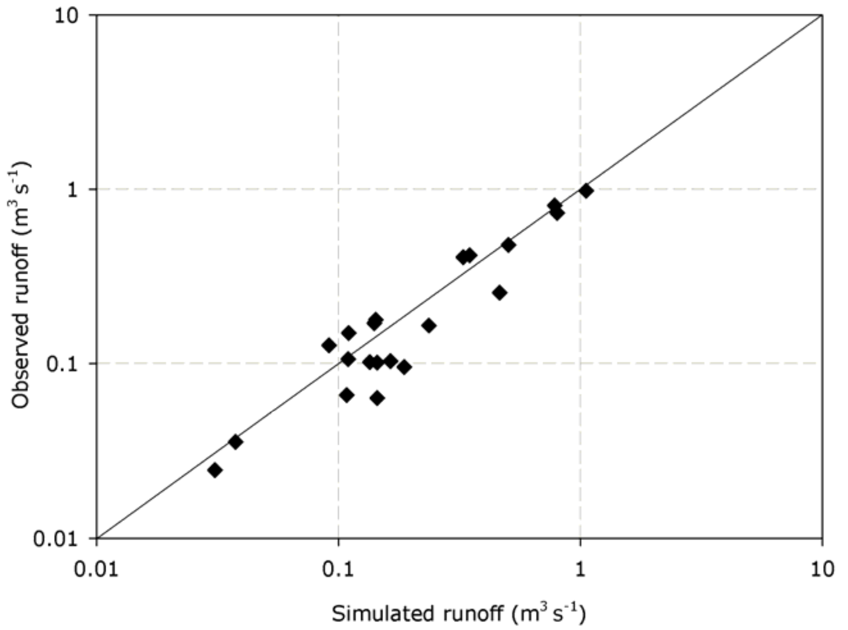

Figure 7.3: Validation of the model performance by comparison of synoptic runoff measurements with simulated discharge.

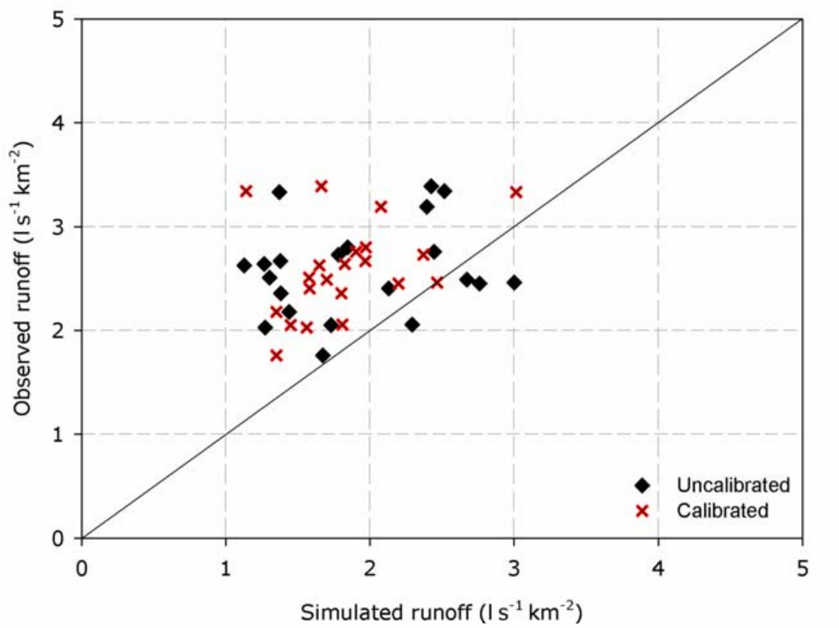

Figure 7.4: Validation of the model performance by comparison of synoptic specific discharge measurements with simulated synoptic discharge.

7.2. Solute transport model

7.2.1. Model calibration

The transport simulation focused on the time period from October 1999 to June 2005 for which extensive data sets were available. Limiting factor for the choice of the application period was especially point source emission data that consisted of time series from 1999 onwards. Diffuse source emissions on the other and were based on leaching coefficients and were not time-dependent in their application.

Calibration of the solute transport model involved only transport related parameters, while the underlying hydrologic model provided hydrologic driving variables based on the best “common” parameter set that was derived by separate calibration of the hydrologic model (cf. 7.1.1). The solute transport model was calibrated against observed Tot-N concentrations that were obtained from the monthly monitoring network of SLU (cf. 5.3.3). Available SLU monitoring stations were located along the main stream network and contained daily Tot-N concentration data in a monthly time resolution for the selected calibration period. Analogue to the hydrologic model calibration, the automated parameter estimator PEST was coupled to the transport model. Subsequent calibration was achieved by minimising the residuals of observed and simulated concentrations in a weighted least square sense.

Due to long model computation times of more than six hours for a single model run, the calibration of the transport model was limited to the period from October 1999 to September 2002 to achieve a realistic time frame for the model calibration. The transport model was initialised by running the model once for the whole application period and by using the obtained model outputs to set the initial solute storages to realistic values. Each model run was preceded by a one-year warming-up period starting from October 1998. The capability of the transport model to capture spatial concentration pattern was assessed by comparing simulated and measured Tot-N concentrations obtained by synoptic sampling (cf. 6.).

7.2.2. Nitrogen transport

Figure 7.5 shows modelled and measured water discharge and nitrogen concentrations in different parts of the Fyrisån catchment for the entire simulation period. It becomes obvious that the concentration dynamic at most stations is commonly related to the discharge dynamic showing high concentration values during spring flood and lower values during summer low-flow conditions. In general simulated nitrogen concentrations reflect the seasonal variation of measured nitrogen concentration. While at some sites the seasonality could be reproduced sufficiently by the model (Flottsund and Klastrop), the model constantly underestimated the concentrations at other sites (Kuggebro) or failed to capture the less pronounced seasonal dynamics (Vattholma). Furthermore it is evident that the model tended to simulate seasonal dynamics in a similar way for most sites (e.g. Vattholma, Klastrop and Kuggebro), although the measured concentration dynamics showed in some cases a more damped characteristic (Vattholma) or a more pronounced variation (Kuggebro). In general long term average concentration levels of Tot-N were matched more sufficiently by the model. In average about 60 % of the variance could be explained by the model (i.e. $R^2 = 0.6$) for calibrated stations.

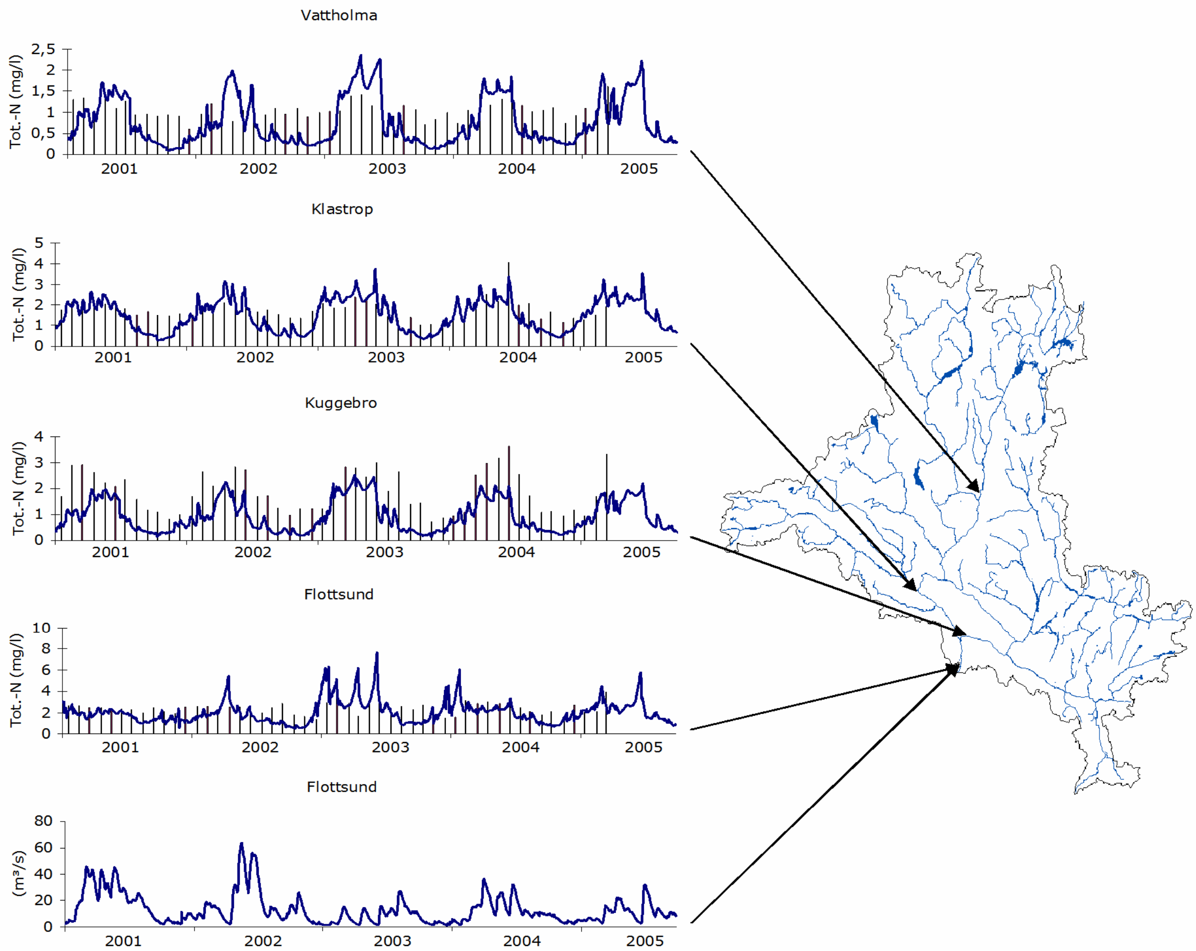

Figure 7.5: Simulated (continuous line) and observed (bars) Tot-N concentrations at selected sites in the Fyrisån and at major tributaries.

7.2.3. Synoptic nitrogen concentrations

The comparison of simulated versus measured synoptic Tot-N concentrations reveals further problems of the model to capture the spatial patterns of nitrogen concentrations adequately throughout the catchment. As the increasing deviation from the 1:1 line indicates in Figure 7.6, higher concentration values were captured more sufficiently by the model, while lower concentration values were constantly underestimated. In contrast to the plotted concentration values, Figure 7.7 demonstrates a homogenisation effect on simulated and observed total nitrogen loads by using modelled discharge values to calculate observed and simulated total nitrogen loads.

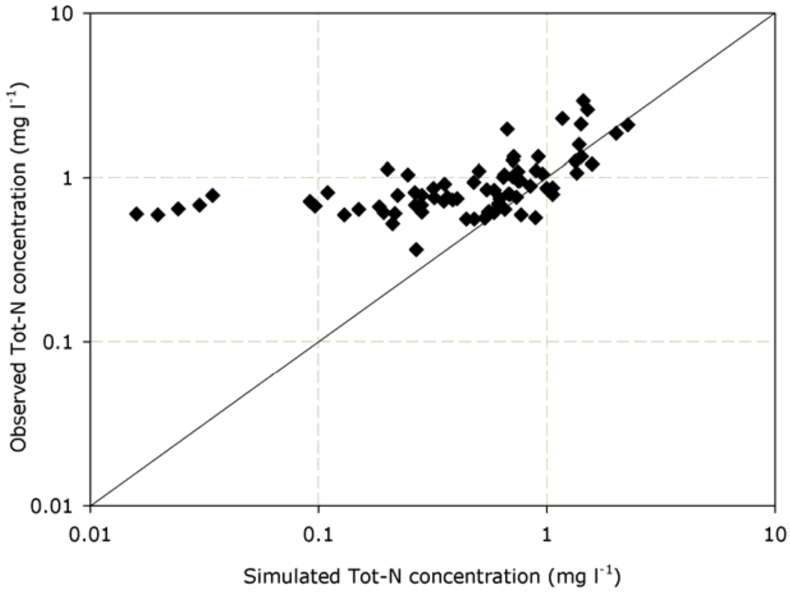

Figure 7.6: Validation of the model performance by comparison of observed synoptic Tot-N concentration with simulated Tot-N concentrations.

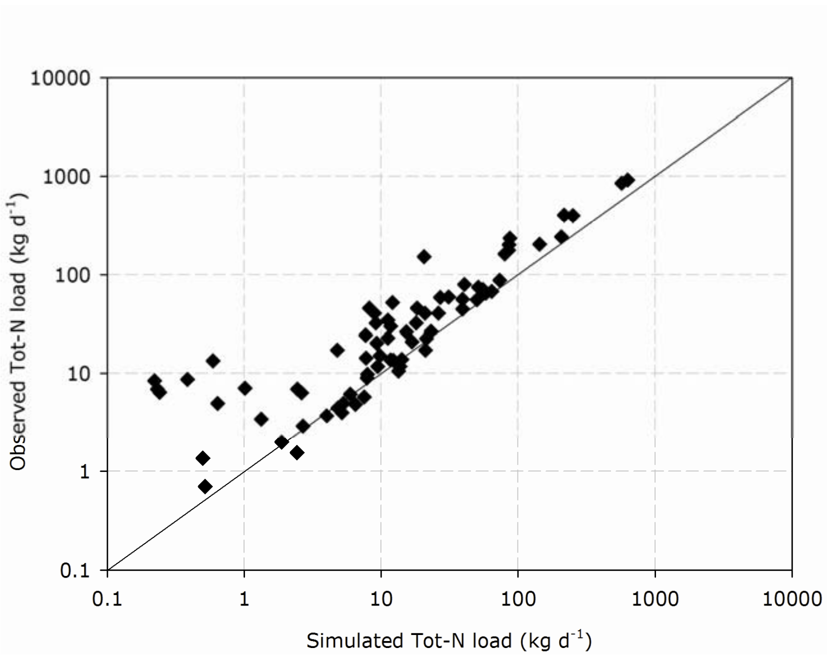

Figure 7.7: Comparison of daily observed synoptic Tot-N loads and simulated synoptic Tot-N loads derived by calculation of modelled discharge at the sample sites.

To assess problem areas and to identify potential relations to distinct land use types, a further analysis of the relative error between measured and simulated Tot-N concentration was carried out. It was found that the relative simulation error depended on catchment size so that with increasing catchment size, the scatter and therewith the relative error was reduced (Figure 7.8). A relation between the relative simulation error and increasing lake percentage was further revealed. Although a large scatter is visible in Figure 7.9, a higher relative error with increasing lake percentage can be identified.

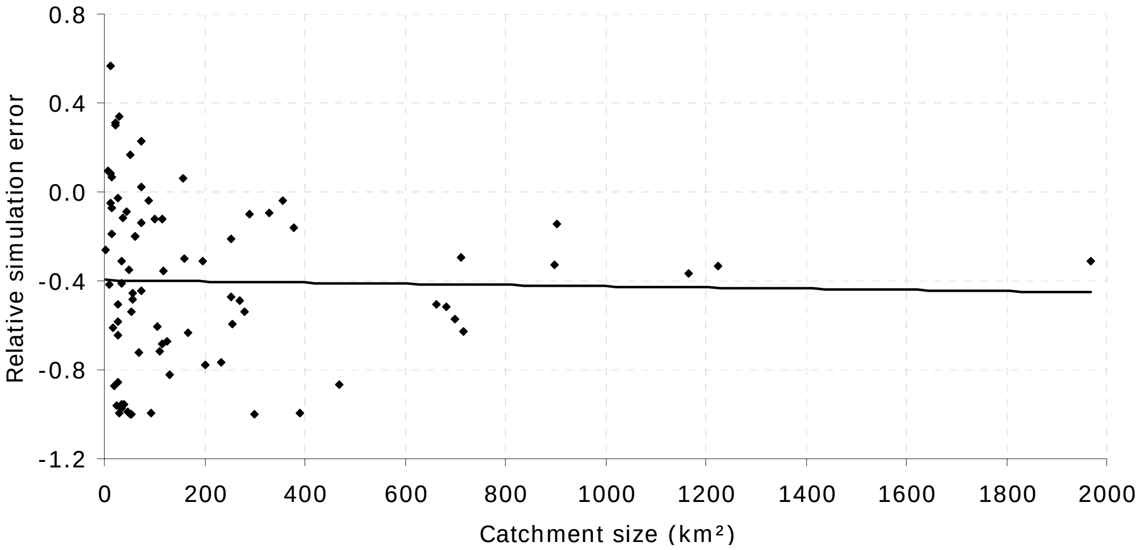

Figure 7.8: Relationship between relative simulation error and catchment size.

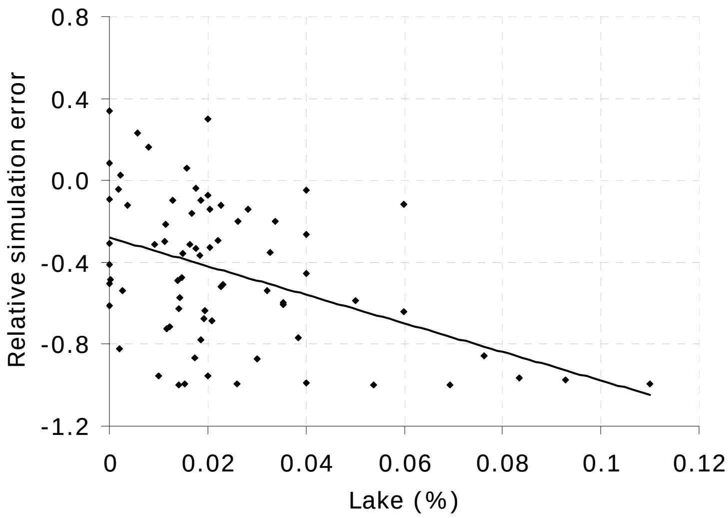

Figure 7.9: Relationship between relative simulation error and lake percentage.

For a further assessment of the modelled spatial evolution of nitrogen concentrations along the Fyrisån, a comparison with measured values of the sampling campaign (Figure 7.10) was conducted. Similar to the prior findings a underestimation of the Tot-N concentration could be found for all sites. This is especially obvious for sites 7, 77 and 50 that are located close to lakes and show almost no nitrogen concentrations. Besides this underestimation, the remaining relative nitrogen concentration dynamic is captured more adequately by the model simulation along the stream.

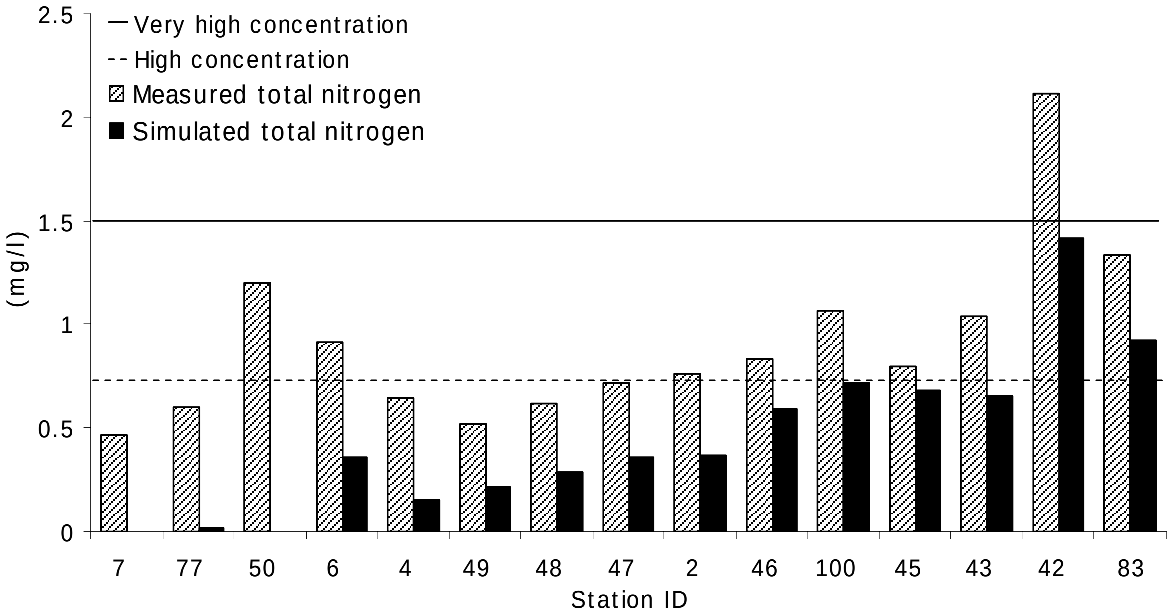

Figure 7.10: Simulated and measured Tot-N concentrations along the Fyrisån.

7.2.4. Source apportionment, retention and scenario runs

Model results presented in this section were based on the parameter set obtained by automated calibration and contain the time period October 1999 to June 2005. Results were calculated for the site Flottsund that is located close to the catchment outlet and thus reflects total loads of the Fyrisån catchment. In studies concerned with nutrient transport modelling, diffuse emissions of nitrogen, such as root zone leakage and point sources are often referred to as gross load, while simulated nitrogen transport after nitrogen transformation in the freshwater system is termed net load (e.g. ARHEIMER 1997). The average total monthly gross load at the site Flottsund was estimated at 118514 kg/month, while corresponding net load was estimated 63139 kg/month for the simulation period (Figure 7.11). The difference between gross and net load constitutes the lumped effect of retention in the catchment and was estimated at 55375 kg/month that corresponds to 46.7 % of the total load.

Source apportionment for each site was achieved by running the model individually for each emission category, while other emissions were “switched off”. The sum of all emission categories constitutes the total net load. Figure 7.12 illustrates the source apportionment at the catchment outlet of the Fyrisån. Leaching from arable land was identified as the largest single source contributing 55.7 % of the Tot-Net load, while point source emissions of water treatment plants contributed 30.2 %. Point source emissions of rural household were only contributing 0.8 %. In addition to the total source apportionment at the catchment outlet, Figure 7.13 presents source apportionment and net loads of Tot-N for major sites along the Fyrisån. For most stations along the stream the dominating influence of arable land is visible. In accordance with results obtained from synoptic sampling and from the SLU monitoring programme, nitrogen loads are generally higher for sites representing sub-catchment areas with intensive farming, while forested regions show comparatively lower loads. But the load calculations also reflect that headwater areas are mostly forested and central parts constitute mainly intensive farm land. Finally a simple scenario run was carried out in order to demonstrate possible application areas of distributed nutrient transport modelling. Figure 7.14

shows the impact of a 50 % reduction and a 100 % increase of water treatment plant emissions across the Fyrisån catchment to the total net load discharging into Lake Ekoln at the catchment outlet.

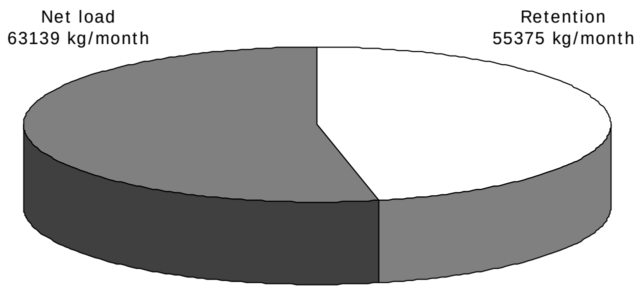

Figure 7.11: Gross load and net load of Tot-N discharging into Lake Ekoln at the Fyrisån outlet.

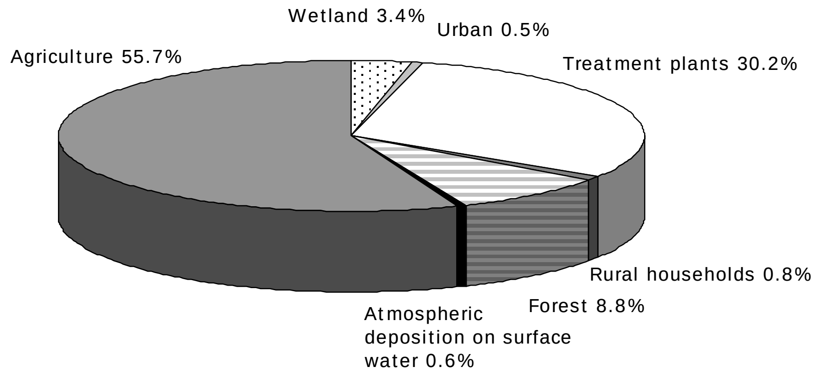

Figure 7.12: Source apportionment of nitrogen net load discharging into Lake Ekoln at the Fyrisån outlet.

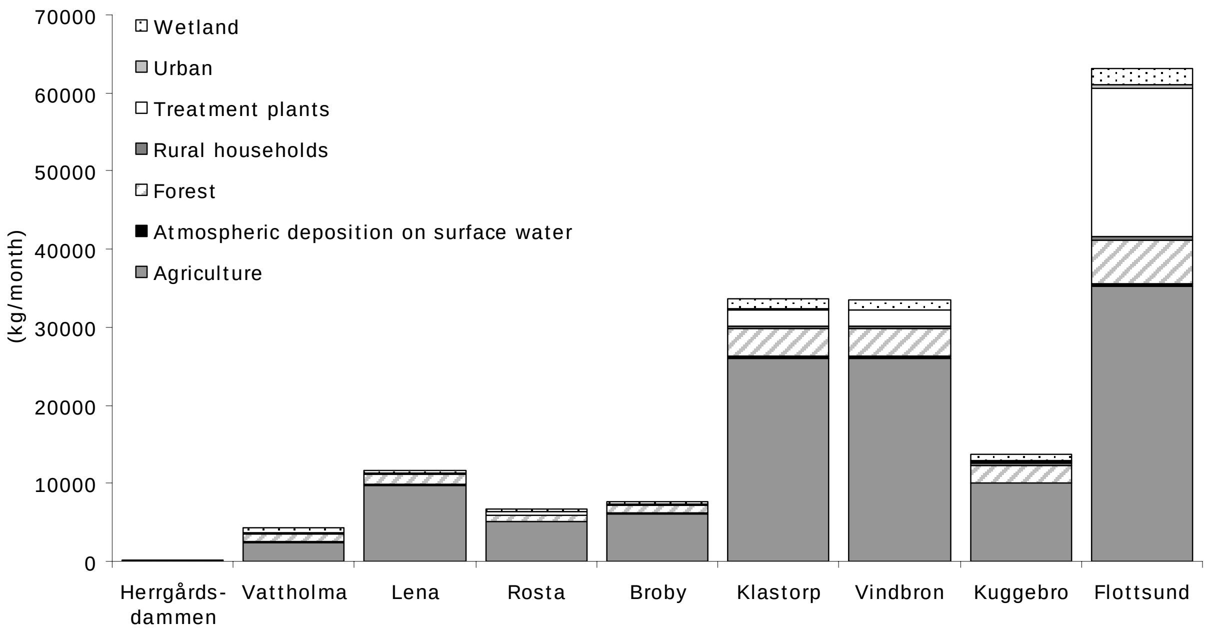

Figure 7.13: Source apportionment and net loads of Tot-N for selected sites along the Fyrisån starting at Herrgårdsdammen and proceeding downstream to Flottsund based on the period 2000 to 2005.

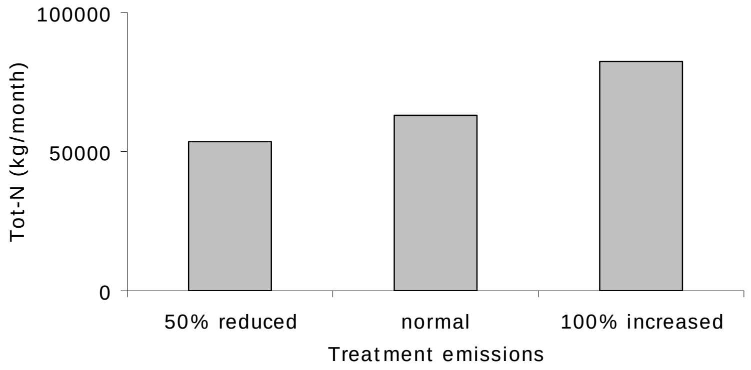

Figure 7.14: Treatment emission scenarios compared to the baseline scenario for the model period 1999 to 2005.

8. Discussion

8.1. Hydrologic model

In general, the intensive model evaluation revealed satisfactory results, but also highlighted some shortcomings that should be critically addressed in the following discussion.

8.1.1. Split-sample test

One major problem to capture adequately the runoff dynamics for certain years was observed for the second half of the Vattholma runoff record. The central cause is probably the clear change in runoff regime from a single spring flow dominated to a more erratic unstable flow regime with multiple peak occurrences. Unstable flow regimes have been noted during former model applications in this region (MOTOVILOV et al. 1999) and have been further investigated by KRASOVSKAIA & GOTTSCHALK (1992) for Scandinavian countries. In this particular case the regime shifts might be also attributed to human influence on runoff formation by dams and weirs at major lakes that trace back to a long mining history in the Vattholma catchment. The resulting poor model simulation that is evident for almost all parameter sets, is most likely a consequence of a too early initialisation of the spring flow by the threshold temperature parameter *TT*. This causes an initial overestimation of the low flow conditions followed by an underestimation of the flood peak volume as exemplarily shown in Figure 7.2. Potential inaccuracies of the model input data (temperature and precipitation) were addressed as a possible factor affecting the model results during this period, but the examination of the respective climate records revealed consistent input data. In this context it should be noted, that the *TT* parameter was apparently adapted well to the more homogeneous training phase with efficiency measures around 0.80 for all applied calibration trials. But based on this under stable conditions derived parameter sets, the model was subsequently incapable to reproduce the different runoff situation of the following time period.

8.1.2. Proxy-basin test

Another issue of the model to account for regional distinctions between the catchments became obvious during multi-scale validation. Although the model incorporates land use dependent runoff generation as well as flow distribution considering spatial information of lakes and streams, it was not able to capture major changes in runoff for different catchments on the basis of an individually calibrated parameter set. This is reflected in low efficiencies for the exchanged parameter sets, especially for the second part of the application period. Here once again differences in runoff regime might play a role, but the computed efficiencies of the measured as well as simulated specific discharges of each catchment indicate a more basic problem: while efficiencies for the measured specific discharges are low signifying considerably different runoff behaviour of the two sub-catchments, the computed efficiencies of the model results are much higher and therewith show that the diverse runoff character was not sufficiently met by the model structure. The fact that the parameter set adapted to one catchment cannot simply be transferred to the adjacent catchments, although the most important spatial processes controlling the flow regime are included, reveals a rather strong dependency on individually calibrated parameter sets in this particular case. This is a strong indication of the “effective” character of these parameter sets that obviously incorporate partly regional spatial heterogeneity characteristics of each catchment.

The simultaneous calibration of the model to both catchments supported this fact with the presence of a “common” parameter set that is able to adequately capture the entire runoff hydrographs for all sub-catchments. It accounts for regional runoff dynamics with a slightly reduced efficiency, but performs much better on an overall basis than both previous individual parameter sets (Table 7.1)

Besides the model application, another often applied approach for runoff predictions in ungauged basins is the transfer of specific discharge from a nearby watershed scaled by the catchment size. This alternative reveals mostly convincing results for catchments with almost identical input data and was compared to the prior model outputs. Table 7.2 reveals a significantly reduced runoff simulation error of the model against a considerably higher bias of the simple transfer method. Due to the almost comparative input data situation for the two basins, the differences in land use and lake distribution are assumed to be the reason for the better model performance. This reflects the value of model applications compared to simpler alternatives, despite the aforementioned deficits to account adequately for most spatial heterogeneity by the model concept.

Besides the model structure, another point in the discussion that needs to be considered is the applied calibration method. Simple lumped models do not suffer from high computation times, so intensive calibration procedures which necessitate many model runs (e.g. Monte Carlo Simulations or Genetic Algorithms) can be easily employed. On the other hand distributed models mostly lack efficiency in computation time and exhibit in most cases even higher parameterisations, due to the complex spatial structures. Therefore less model runs for calibration purposes are possible and the optimal “global” parameter set is not inevitably achieved every time. This fact might be underestimated, but could be clearly verified on the basis of different start parameters for the coupled parameter estimator PEST. It was found that the variation of initial parameters resulted in different optimised parameter sets with varying model performances. This showed besides the well known problem of equifinality (e.g. BEVEN 2001) that the optimisation algorithm of PEST was apparently not able to find a “global” parameter set, but obtained the next best “local” parameter set instead.

8.1.3. Model comparison

By further comparing the HBV model with the distributed model, it was shown that the latter did not lead to any sufficient improvement of the discharge simulation capabilities over the much simpler lumped model approach. Both models proved to be more or less equivalent successful in simulating discharge for the different catchments and performing equally well in split-sample and proxy-basin tests. Therefore both models access the same fundamental model theory and equations. Major differences in the model structures are in general based on the treatment of data in a lumped or distributed manner resulting in the special adaptations of the distributed model outlined at the beginning of this study.

However, these findings were not anticipated beforehand. Particularly with regard to the transfer of model parameters to adjacent catchments, it was expected that the distributed model performance would be superior due to the consideration of major spatial hydrological processes dominating in each region as well as the increased degree of freedom. But after intensively evaluating and comparing both models in this study it has to be frankly stated that the lumped model concept, in terms of discharge simulation at the catchment outlet, is even slightly superior to the distributed model results. With respect to the classic argumentation about the value of distributed versus lumped modelling (e.g. BEVEN 1996; REFSGAARD et al. 1996) this model comparison may be therefore seen as an basic example for the supremacy of less parameterised lumped model concepts, if the objective is the best discharge fit at the catchments outlet. As pointed out in this discussion and by several authors (e.g. BEVEN 2001; SEIBERT 1999a), distributed models can seldom demonstrate to be superior to much simpler lumped or semi-distributed models, if only tested against runoff at the catchment outlet that constitutes "lumped" data, integrated over the whole catchment. In contrast, the main advantage of a distributed model is its capability of simulating "more" than just runoff with various internal state variables that can be subject to multi-criteria calibration, if additional data is available. This is especially important in terms of evaluating model structure uncertainty and refining hydrological process descriptions in order to prevent the "*we are right for the wrong reasons*" case (KLEMES 1986) to which lumped model concepts may tend to.

In view of this the advantage of the process-oriented runoff generation routine shall be pointed out as an example for the different internal state variables that are simulated within the applied model. It can be exemplified by the individual runoff response per land use class for headwater cells in the Fyrisån catchment. Table 8.1 shows that the average daily storage outflow of headwater grid cells corresponds to the predominating land use distribution.

Table 8.1: Computation of mean daily storage outflow of headwater grid cells in the Vattholma catchment.

Storage Type Outflow	Forest	Agriculture	Urban	Wetland
Upper Storage (mm d^{-1})	0.098963066	0.01744986	0.00042701	0.007896214
Lower Storage (mm d^{-1})	0.00450366	0.00008960	0.00000526	-

Thus forest contributes most to lateral runoff generation, followed by agriculture, wetland, and settlements. Nevertheless, if one looks at the single land use cells it becomes obvious that besides this spatial aggregation effect the individual cell runoff dynamic can be different. In this case for example the agricultural land use class was assigned the highest outflow recession coefficient, while at the catchment outlet forest was the dominating land use class in terms of runoff generation. Depending on the location within the catchment and the surrounding land use the individual runoff response is superimposed and thus reflects the response of a certain larger area. In some respect a scaling effect of runoff response is therefore implicitly reproduced by the distributed model which is impossible for lumped model concepts. Such spatial differentiated simulations are essential for the next step towards integrated catchment modelling with further inclusion of solute transport process into model structures. In particular with respect to solute transport models, it means a great improvement to include a spatial representation of solute transport processes based on a detailed description of hydrological flow processes. Point sources and diffuse sources can be incorporated according to their spatial representation so that degradation and retention can be simulated in a more process-realistic way.

In this context, the application of the sub-grid parameterisation scheme is beneficial. Especially in situations where models with a rather coarse grid resolution need to consider small scale processes in an adequate manner with limited computation power. This is frequently the case at larger scales such as Regional Climate models with Land Surface Schemes (e.g. KOTLARSKI & JACOB 2005) or Soil-Vegetation-Atmosphere-Transfer (SVAT) models (e.g. STRASSER & ETCHEVERS 2005), but can be also transferred to mesoscale model applications like nutrient transport modelling, where small lakes, wetlands or riparian zones can have a considerable impact on nutrient flows and distributions (CARPENTER et al. 1998; GREN 1995; HOOPER 2001).

8.1.4. Synoptic runoff measurements

Model evaluation based on synoptic runoff measurements demonstrated to be valuable tool for a thorough model testing procedure, in particular with regard to the model capability for distributed runoff predictions. It has the advantage to gain supplementary data for model evaluation purposes with comparatively little time and effort compared to measurements of other hydrological variables. One snapshot campaign during low flow conditions is certainly not enough to draw a representative conclusion, but the results give an indication that the applied model has problems to capture adequately the spatial pattern of stream flow at a specific date. The results from the calibration effort of the model on the synoptic discharge measurements are in line with these findings and confirm that the flow and river routine is obviously not capable to reproduce the diverse runoff pattern throughout the catchment accurately at this specific date. A variety of reasons might come into play. One factor affecting results might be that the measurements were instantaneous while the model simulations are performed in a daily resolution and therewith describe the average flow conditions. Although low flow conditions are rather stable (i.e. no pronounced daily discharge fluctuations) and more easily to reproduce by the model, small effects can have bigger impact on flow conditions such as human regulation or increased measurement bias. Another factor could be inaccuracies in the spatial delineation of the local drain direction network or within the flow routine itself. This is very likely considering the difficulties to derive a good flow direction network in this catchment (cf. 5.1.1). A significant flow component is also happening in the subsurface in the flat study area, maybe bypassing the synoptic sampling locations. The flow direction is also often not defined by the surface topographic gradient, what makes the check of distributed surface runoff predictions with such data sets even more difficult. Consequently, more synoptic measurement campaigns would be certainly helpful to gain consistent data and further address these issues.

8.2. Solute transport model

Modelling of nitrogen transport is associated with large uncertainties due to the complex processes involved. The obtained model results reflect this uncertainty to a large part and are subject to further discussion in the following paragraphs.

8.2.1. Model uncertainty

The nitrogen transport model application was based on a large data set including simulated concentrations from root zone leakage for several land use types, point source emissions of water treatment plants, and rural households as well as atmospheric deposition on open water courses. Model results reveal that the general spatial nitrogen concentrations patterns and seasonal variability could be reproduced, while simulations of more detailed temporal and spatial Tot-N concentrations were not convincing for all stations.

As mentioned before, water quality modelling depends largely on the quality of the input data, as it has direct effect on modelled concentration. Although the most detailed data available was used in this study, still a large source of error and uncertainty can be related to the input data. The utilised standard leakage coefficients may not be representative for each land use situation, since these coefficients reflect average long-term outputs of the SOIL-N model system for monoculture crop growth and constant fertilisation regimes. Although these coefficients were related to the most detailed available crop growth and field parcel data base, the data base reproduced only the distribution and crop types for a specific year and thus changing crop and fertilisation regimes may induce a different seasonal variability. Since only constant leaching coefficients were available for other land use forms and concentration dynamics from watersheds with mixed land use and arable land do not show the same distinct seasonality, this could be one factor affecting the models capability to capture different seasonality of Tot-N concentrations across the catchment based on land use distribution. Besides diffuse sources that constitute by far the major part of the nitrogen load at the catchment outlet, point source emissions are also subject to uncertainty. Detailed data was only available for water treatment plants in the drainage basin and was disaggregated to a daily time step for most stations, while detailed information about industrial sewage emissions was lacking. It became obvious during synoptic sampling that point source emission may have substantial impact on water quality and industrial source emissions might contribute to in-stream nitrogen variations. Also the disaggregation of weekly, biweekly or monthly data might neglect the dynamic caused by these emissions.

In terms of calibration data, the obtained concentration measurements of the SLU monitoring network may be of different quality for different years, since analysis methods have changed over time (e.g. Tot-N in 2002). Moreover the mostly monthly or biweekly sampling may not capture the variability of stream chemistry entirely, especially during spring flood with different mobilisation processes involved.

In addition to uncertainty related to input data, the structure and routines of the applied model may be erroneous. A thorough analysis of the spatial pattern derived from the synoptic sampling campaign revealed problems with the lake routine of the model. The correlation between measured and simulated concentration showed an increasing error towards low concentration values for catchments with high lake percentages reflecting a problem of the model to capture low concentration ranges adequately. The prominent outliers in Figure 7.6 were identified as sample sites located direct downstream of lake outlets. The more detailed analysis revealed that lake retention in the model simulation was too high under the low-flow conditions of the sampling campaign resulting in the underestimation of concentration values as seen in Figure 7.3 and along the stream profile for sites 7, 77 and 50. The further analysis also indicated that the simulation of small headwater sub-catchments is not well captured by the model in most cases, while with increasing catchment size the error was considerably reduced reflecting the more homogenous reaction of large areas in which small scale effects might cancel each other out. This problem of the model to capture the spatial pattern of certain variables was already discussed for the hydrologic model and thus it is not surprising to find even higher errors for the concentration simulations, since the nutrient transport simulation was based upon the hydrologic driving variables. But even though absolute concentration calculations might not be correct for all sites, the relative differences between concentrations are more reliable (Figure 7.10), since a detailed representation of the landscape mosaic favours a more realistic distribution of point and non-point sources as well as retention in comparison to simpler lumped models.

A further problem of the model was the adequate representation of the heterogeneous seasonal concentration dynamic. It can be partly addressed to the input data as discussed before, but seems also a result of the applied retention functions. These retention functions represent the lumped effect of different nitrogen fractions and thus suffer from a reduced flexibility to adapt to different concentration dynamics. This is especially important, as it was shown that the organic nitrogen fraction was dominating in the Vattholma sub-catchment and nitrate and nitrite dominated the central parts of the Fyrisån. A further limitation of the retention function is the strong correlation to temperature reducing the ability of the model to adapt to heterogeneous concentration variation across the catchment. In particular the assumption that no retention occurs below 0°C might be questionable, since adsorption processes may persist during winter time. From a conceptual perspective it is a further limitation to the flexibility of the retention function implying that the modelled gross load level during winter is sufficiently reproduced only by the used input data. Hence the mathematical construction of the function might be subject to further improvements to increase its flexibility in order to allow a better adaptation to distinct seasonal variation. Moreover calibrated model parameter may also be erroneous, since they could not be calibrated separately and reflect the lumped effect of retention occurring in the water bodies of groundwaters, rivers, and lakes.

In general, the model performance corresponded to results typically seen from nutrient transport models in Nordic environments (e.g. ARHEIMER 1998; DARRACQ et al. 2005; KVARNÄS 1996) and reflects the level of uncertainty that is typically associated to model applications at this scale and time resolution. The comparison of the derived model results with models applied to the Fyrisån is difficult due to the different application periods and calibration methods that were used. A further comparison between models based on performance measures might be also problematic, as model performance in several studies was often judged by comparing calculated and measured loads based on monitored concentrations. This is misleading due to the dominating influence of runoff on load calculations. It is even more misleading if the same (simulated or observed) runoff is used for the computation of loads, as nutrient transport depends largely on discharge variability and a model assessment based on loads derived with the same discharge values reduces the degree of freedom considerably and thus pretends a better model performance. This effect is exemplarily expressed in Figure 7.7 for loads derived with the same modelled discharge values. Although the deviation form the 1:1 line remains for low discharge values in this example, it becomes obvious that the range of obtained values is significantly increased. This implies a better overall correlation, what is in fact caused by discharge varying with the respective sub-catchment size. Unfortunately this procedure is found in several studies and can be regarded as inappropriate for an evaluation of the model performance. Consequently a thorough model evaluation should be based on temporal and spatial concentrations values of water quality parameters instead of loads.

8.2.2. Source apportionment, retention and scenario runs

Distributed solute transport modelling offers the possibility for a detailed analysis of modelled nitrogen loads and concentrations. It allows the identification of problem areas and helps to develop remedial measures to reduce nitrogen loads in order to fulfil European Water Framework Directive requirements. Although uncertainties within this model approach are comparatively large, the analysis of model results at the outlet of the River Fyrisån intends to give an impression of the potential of distributed water quality models. The analysis focused mainly on the site Flottsund, located at the catchment outlet, where simulation results were regarded as sufficient and a catchment-wide assessment of nitrogen loads and contributions to Lake Ekoln and the Lake Mälaren system was feasible.

As pointed out in the previous discussion, it is difficult to compare studies that are based on different data bases, since the utilised data sources determine to a large degree the simulation results. Also hydrological and climatological conditions differ mainly due to different application periods and resolutions employed by different model concepts. However, model derived long term estimates and load calculations may be compared and might give an indication of the reliability of the model results. For this reason key model outputs were compared briefly to available model results derived by the conceptual lumped Fyrisån model (KVARNÄS 1996) that was applied to a simulation period from 1989 to 1994.

Hence it was found that average retention values obtained during this study (47 %) corresponds largely to the estimated average retention derived by the Fyrisån model (49 %) and is also in line with computations of the average retention ranges in south Sweden (ARHEIMER 1998). In contrast, the modelled average net load of Tot-N, derived by the both models for the different time spans, differed significantly between 70390 kg/month for the Fyrisån model and 63139 kg/month for the current model approach. However, inter-annual variations of loads are substantial ranging from 54623 kg/month (1989) to 87612 kg/month (1990) for calculations of the Fyrisån model. In consideration of the different model application time periods, these results imply that both models simulate the long term average nitrogen loads on a similar level. A significant difference was evident for the source apportionment. The Fyrisån model revealed a Tot-N contribution at Flottsund of 66 % for treatment plants and only 26 % for arable land, while in the current study opposite values of 56 % for arable land and 30 % for treatment plant Tot-N contribution could be found. The gradual improvement of the water treatment plant in Uppsala resulted in lower nitrogen emissions since 2000 and might explain a small part of the decrease of the treatment plant contribution. Also different input data bases certainly play a role and call for a further model assessment based on the same model inputs. Besides the rather large impact of the water treatment point source emissions, contributions of rural household emissions to the total net load at the Fyrisån outlet were small, although local differences might exist, but were not further evaluated during this study.

The comparison of nitrogen source apportionment for different stations along the stream revealed the main influence of agricultural leaching for all sites throughout the catchment. Moreover it pronounces the influence of the impact of the water treatment plant in Uppsala on water quality at the Fyrisån outlet in Flottsund. A simple scenario analysis was carried out and revealed that a 50 % reduction of water treatment source emissions across the catchment would reduce the average monthly load at the site Flottsund about 10000 kg/month. This is almost exactly the half of the Uppsala water treatment plant emissions revealing that remediate measures across the catchment would have probably little effect on the outlet water quality. The exact opposite behaviour was estimated for a doubled emission scenario. This demonstrates that information about spatial distribution of nitrogen transport can indicate where remedial measures could be established across a catchment and in combination with estimates about source apportionment, this could provide essential information on which sector measures should be implemented.

9. Concluding remarks

9.1. Hydrologic model

In this study a model application to the Fyrisån catchment with adequate model performance for different sub-catchments for the calibration and the validation period was achieved. A conceptually reasonable simulation of spatial distributed hydrologic conditions in the Fyrisån catchment could be realised by a land-use based runoff generation routine. A sub-grid parameterisation scheme allowed a correct representation of small scale land-use patterns within the catchment area, such as wetlands, while a flow routing and lake routine captured runoff dynamics adequately. However, a detailed assessment of the flow distribution and retention routine was not possible, since detailed runoff records at lake in- and outlets were not available. Hence a conceptual and fully distributed simulation of the hydrologic conditions in the Fyrisån catchment could be established. This refined model concept offered a link to the further incorporation of solute transport routines, where realistic hydrological modelling is the prerequisite for water quality modelling.

In the course of the intensive model evaluation and comparison also shortcomings of the model capabilities became evident and should not be neglected. The model failed to capture the runoff dynamics adequately for certain years of the simulation period. Different parameter sets were derived by calibration, but with none of these the model was able to achieve better runoff simulations solely by integrating additional spatial information. Moreover the model performed equally well than the much simpler lumped HBV model with regard to simulating runoff. Also the model had obvious problems to reproduce the spatial variation in runoff sufficiently in comparison to synoptic runoff measurements.

It is important to note that the identification of these problems was only possible due to the rigorous tests that were carried out during the model evaluation process. This clearly reveals the importance of a thorough model evaluation procedure. Besides the already well established test procedures described by KLEMES (1986), it was demonstrated that the comparison with hydrologic benchmark models, such as the HBV model, is crucial to gain further knowledge and to draw further conclusions about the model performance.

Additionally problems concerning evaluation of distributed models against runoff measurements at the catchment outlet were addressed and highlighted once more the need for additional data to evaluate and demonstrate the benefit of the distributed model concepts. In this regard synoptic stream flow measurements proofed to be an efficient tool to provide additional data for a thorough model evaluation by adding a spatial component into the evaluation process that is normally focused on time series at a few locations throughout the catchment, i.e. the temporal aspects of runoff.

9.2. Solute transport model

The implementation and evaluation of a nitrogen transport routine coupled to the developed hydrological model, as a main objective of this study, could be achieved. The model enables, in contrast to lumped model concepts, both temporal and spatial nitrogen concentration simulations in a fully distributed manner. Realistic and detailed nutrient transport simulations depend thereby largely on the quality and amount of available input data. Hence, the collection, procession, and allocation of comprehensive spatial and temporal input data in a central data base were a main prerequisite for the model application within the scope of this study. A synoptic sampling campaign was carried out and helped to gain further insight into the spatial distribution of nutrients across the catchment and enabled additional model evaluation. This work resulted in the most detailed data set for nutrient transport applications in the Fyrisån region.

The transport model was calibrated against monthly concentration values of total nitrogen and the obtained simulation results were poor for some stations and also intensive model testing revealed different problem areas. Especially the retention equations which were taken from the HBV-N model were identified as a conceptual limitation to adapt the model to the dynamic seasonal variation at different sites throughout the catchment. Similar to the hydrologic model, deficits in the simulation of the spatial nutrient concentration patterns were found. In particular the conceptualisation of lake retention was identified to lead to an underestimation of nitrogen concentrations during low-flow periods.

The further analysis of the derived model outputs allowed a brief comparison to other model results and demonstrated the potential of nutrient transport models to assess water quality problems and enable an efficient watershed management, if the level of uncertainty is considered. The comparison showed a general agreement in average long-term gross and net loads, while source apportionment revealed major differences. Nevertheless, a further assessment of model outputs calls for a detailed comparison based on the same data base. Against the background of theses results it is argued that the model approach presented in this study shows a similar performance than comparative models, where intensive and critical model testing is often omitted and the level of uncertainty involved in the simulation is often not clearly stated.

9.3. Outlook

A distributed nitrogen transport model was developed and applied to the Fyrisån catchment. The developed model and the obtained comprehensive data sets can be seen as a framework for further research activity in the Fyrisån catchment.

A further collection of allocation of data is certainly needed to gain more insight in potential problem areas and to enable more detailed model applications. In particular a second synoptic sampling campaign would be beneficial, as it helps to constrain available data and allows a further statistical analysis. In view of this, the additional inclusion of sampling parameters such as N^{15} may help to identify source emissions and to further refine model concepts. In combination with the available synoptic data, the already available data sets constitute a comprehensive data pool with detailed and long chemical, hydrological and, meteorological records that are rarely found in mesoscale basins. This would allow establishing the Fyrisån catchment as a benchmark basin and enables the comparison of different model types based on the same consistent input data.

The further development of the applied distributed model; based on the critical model evaluation in this study; could help to reduce the model uncertainty and allow more reliable model results. In particular the implementation of other fractions of nitrogen and in a next step the implementation of phosphorous would be beneficial. It would enable more detailed scenario and water management related model applications in order to identify potential water quality problems and help to implement remedial measures against the background of the implementation of the European Water Framework Directive.

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Appendix

Precipitation stations

Name of station	Coordinate RAK X	Coordinate RAK Y	Level (m a.s.l.)	Precip. from	Precip. to
Vattholma	6657490	1607150	25	01.01.1961	30.06.2005
Harbo	6669440	1579450	40	01.04.1975	30.06.2005
Films Kyrkby	6681560	1616290	39	01.02.1982	30.06.2005
Risinge	6675330	1634230		01.02.1962	30.06.2005
Uppsala	6639020	1601800	21	01.01.1961	30.06.2005
Drälinge	6653840	1598510	30	01.01.1961	30.06.2005
Almunge	6648160	1625300		01.05.1988	30.06.2005
Vällnora	6651220	1641760		01.04.1970	30.06.2005

Climate stations

Name of station	Coordinate RAK X	Coordinate RAK Y	Temp. from	Temp. to
Films Kyrkby	6681560	1616290	01.02.1982	30.06.2005
Risinge	6675330	1634230	01.02.1962	30.06.2005
Uppsala Flygplats	6643060	1599910	01.01.1961	30.06.2005

Discharge stations

Name of station	Coordinate RAK X	Coordinate RAK Y	Runoff from	Runoff to
Vattholma N. Bro	6657200	1607380	01.01.1979	30.06.2005
Sävjaån	6635920	1606520	06.09.1979	30.06.2005
Ulva Kvarndamm	6645090	1599020	12.09.1979	31.12.1999

SLU monitoring stations

Name of station	Station ID	Coordinate RAK X	Coordinate RAK Y	Chemistry from	Chemistry to
Vattholma N. Bro	1	6657200	1607380	15.01.1991	14.12.2004
Jumkilsån Kallön	2	6655570	1578980	16.01.2004	15.12.2004
Tobo Reningsver.	3	6683450	1603100	12.09.2001	14.12.2004
Tobo Bruksgatan	4	6683950	1602700	12.09.2001	14.12.2004
Vendelsjön	5	6672180	1601020	22.04.1998	28.08.2001
Fyrisån St Eriks	6	6641040	1600800	21.02.1994	16.12.1996
Fyrisån Ulva Kvarn	7	6645160	1599050	21.02.1994	16.12.1996
Västra Ekeby	8	6669330	1599860	15.01.1991	16.12.1996
Lena Kyrka	9	6656220	1606680	15.01.1991	14.12.2004
Vindbron	10	6636140	1604100	15.01.1991	14.12.2004
Fyrisån Klastorp	11	6642140	1599290	15.02.1965	14.12.2004
Fyrisån Flottsund	12	6631160	1604150	15.01.1965	14.12.2004
Lötsjön	13	6638940	1619260	22.04.1998	28.08.2001
Funbosjön	14	6639580	1615110	22.04.1998	28.08.2001
Gruvkanalen	15	6676900	1612900	13.03.2001	03.03.2004
Filmsjöns utlopp	16	6679300	1615450	13.03.2001	03.03.2004
Dalån	17	6675450	1613850	13.03.2001	03.03.2004
Slagsmyren	18	6671800	1616600	13.03.2001	03.03.2004
Harvikadammen	19	6675300	1614600	13.03.2001	03.03.2004
Sävjaån Ingvasta	20	6656490	1613970	18.01.1965	14.12.2004
Sävjaån Lejsta	21	6650250	1617050	18.01.1965	16.12.2003
Sävjaån Kuggebro	22	6636170	1605790	18.01.1965	14.12.2004
Broby	23	6643400	1597280	15.01.1991	16.12.2003
Rosta Kvarn	24	6649160	1600880	15.01.1991	16.12.2003
Herrgårdsdammen	25	6676980	1616220	15.01.1991	16.12.2003
Viken	26	6668510	1609540	15.01.1991	17.01.2000
Stordammen	27	6677960	1618840	13.05.1969	03.03.2004
Dannemorasjön	28	6674600	1612560	13.05.1969	03.03.2004
Siggeforasjön	29	6651750	1575590	08.08.1983	17.10.2004
Edasjön	30	6633650	1617790	02.08.1983	28.10.2004

Sewage treatment plants

Name of station	Coordinate RAK X	Coordinate RAK Y	Emissions from	Emissions to
Gunsta	6639350	1613470	01.01.1995	31.12.04
Jälla	6642660	1607720	01.01.1995	31.12.04
Uppsala	6637300	1603780	01.01.1995	31.12.04
Länna	6642050	1621530	01.01.1995	31.12.04
Gåvsta	6650050	1616380	01.01.1995	31.12.04
Storvreta	6650530	1604950	01.01.1995	31.12.04
Björklinge	6657000	1596350	01.01.1995	31.12.04
Skyttorp	6663270	1608230	01.01.1995	31.12.04
Vattholma	6656120	1607220	01.01.1995	31.12.04
Husby	6671270	1598650	01.01.1995	31.12.03
Dannemora	6679300	1615500	01.01.1995	31.12.04
Örbyhus	6679950	1605700	01.01.1995	31.12.03
Tobo	6683900	1602700	01.01.1995	31.12.03

Laboratory measurement methods and ranges

Analysis variable	Method (reference)	Measurement error (%)	Measurement range
TOC	SS-EN 1484	6	0.3-50 mg/l
Aluminium	SS-EN ISO 11885	8	5-2000 µg/l
Iron	SS-EN ISO 11885	5	5-2000 µg/l
Silicate	Bran Luebbe Industrial method No. 811-86T	9	0.5-8 mg/l
pH	SS 028122-2 mod	2	3-10
Conductivity	SS-EN 27888-1	3	0.1-100 mS/m
Calcium	SS-EN ISO 11885	5	0.001-5.0 mekv/l
Magnesium	SS-EN ISO 11885	5	0.001-1.0 mekv/l
Sodium	SS-EN ISO 11885	5	0.001-3.0 mekv/l
Potassium	SS-EN ISO 11885	5	0.0005-0.3 mekv/l
Alkalinity	SS-EN ISO 9963-2 mod	4-8	0-1 mekv/l
Acidity	American Public Health Association (1985)	10-14	0-0.100 mekv/l
Sulfate	SS-EN ISO 10304-1 mod	6	0.01-1.7 mekv/l
Chloride	SS-EN ISO 10304-1 mod	8	0.004-0.6 mekv/l
Fluoride	SS-EN ISO 10304-1 mod	6	0.02-4 mg/l
Ammonium nitrogen	Bran Luebbe Method No.: G-176-96 for AAIII	10-35	2-100 µg/l
Nitrite + nitrate nitrogen	SIS 028133-2 mod Bran Luebbe Method No.: J-002-88B	10-20	1-700 µg/l
Kjeldahl nitrogen	SIS 028134-1 mod	10-20	50-1000 µg/l
Tot-N	SS-EN ISO 11905 mod Bran Luebbe Method No.: J-002-88B	10-20	50-4000 µg/l
Phosphate phosphorus	Bran Luebbe Method No.: G-176-96 för AAIII	8-19	1-25 µg/l
Total phosphorus	SS 028127-2 mod Bran Luebbe Method No.: G-176-96 för AAIII	20-35	2-50 µg/l