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The model ForSAFE-2D
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Modelling nutrient transport from forest ecosystems to surface waters

The model ForSAFE-2D

Giuliana Zanchi

DOCTORAL DISSERTATION
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Abstract
Forests provide multiple products and services which are all are linked to water resources. Trees need water to grow and, at the same time, they change the quality and the quantity of runoff by modifying water and nutrient cycling. The understanding of the interactions between forest and water is fundamental to assess the consequences of natural and anthropogenic pressures, such as climate change and forest management, on the provision of forest products and services. Due to the complexity of ecosystems, models are often used to understand the interactions between different system components under a changing environment. ForSAFE is a dynamic, mechanistic ecosystem model simulating the storage and fluxes of chemical elements in forest ecosystems. It was developed to better understand the effects of environmental changes on the chemistry of forest biomass, soil and soil water at the forest plot level. The first two studies in this thesis are examples of the application of ForSAFE in forest stands in Southern Sweden. The model is used to simulate the effects of anthropogenic and natural disturbances on different ecosystem indicators, including indicators of soil water quality. The studies show that nutrient leaching below the rooting zone is positively related to the nutrient availability at the site, soil disturbances and the amount of organic material left in the forest after tree felling or a storm. Both types of disturbance produce a temporary increase of the acidity of the soil solution, but long-term effects where not predicted by the model. Compared to harvesting, a higher nutrient release in the soil solution can occur after storms due to root lifting causing increased mineralization, a larger amount of biomass left at the site due to technical and economic constraints and larger canopy openings. In addition, sea-salt episodes can increase the acidity of the soil solution in the first years after the storm. When considering other ecosystem services, trade-offs can exist between the reduction of nutrient loads in the soil solution and the accumulation of carbon in the forest. The conclusions drawn from the application of ForSAFE at the forest plot level are valid for the soil water chemistry in the unsaturated zone. In this thesis, an effort has been made to expand the model simulations from the plot to the hillslope scale to understand how forest ecosystems can affect the chemistry of the streams. A new hydrology concept was integrated in ForSAFE-2D that simulates two-dimensional flows of water and chemical elements from the forest to the stream. ForSAFE-2D allows a better representation of the moisture content by simulating an increasing water saturation level in deeper soil layers and towards the stream. The simulated transport of a tracer along a hillslope shows that the model is capable of capturing the average concentrations of the tracer in the stream. This capability is based on a correct representation of the long-term average runoff and of tracer concentrations in the soil solution. The results also highlight some of the issues that should be addressed by follow-up research studies. The partitioning of water between base flow and peak flows suggests that the simulation of flow paths by ForSAFE-2D should be re-evaluated. A correct representation of flow paths will be crucial when simulating the transport of elements or compounds which change concentration with depth or distance from the stream (e.g. dissolved organic matter). In addition, the effects of saturation on weathering, as well as decomposition, show that the regulation of these processes at increasing moisture contents should be updated. Finally, the process regulating the allocation of carbon and nutrients to foliage should be revised to increase the share of foliage in the tree biomass and thereby correct the simulation of evapotranspiration.

Key words: forest, dynamic modelling, hydrology, biogeochemistry, ecosystem service

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Modelling nutrient transport from forest ecosystems to surface waters

The model ForSAFE-2D

Giuliana Zanchi

LUND UNIVERSITY
To my future: Gerben and Teresa
And to my roots: mamma e papá

Reality: what a concept!
(Robin Williams)
Abstract

Forests provide multiple products and services which are all are linked to water resources. Trees need water to grow and, at the same time, they change the quality and the quantity of runoff by modifying water and nutrient cycling. The understanding of the interactions between forest and water is fundamental to assess the consequences of natural and anthropogenic pressures, such as climate change and forest management, on the provision of forest products and services.

Due to the complexity of ecosystems, models are often used to understand the interactions between different system components under a changing environment. ForSAFE is a dynamic, mechanistic ecosystem model simulating the storage and fluxes of chemical elements in forest ecosystems. It was developed to better understand the effects of environmental changes on the chemistry of forest biomass, soil and soil water at the forest plot level.

The first two studies in this thesis are examples of the application of ForSAFE in forest stands in Southern Sweden. The model is used to simulate the effects of anthropogenic and natural disturbances on different ecosystem indicators, including indicators of soil water quality. The studies show that nutrient leaching below the rooting zone is positively related to the nutrient availability at the site, soil disturbances and the amount of organic material left in the forest after tree felling or a storm. Both types of disturbance produce a temporary increase of the acidity of the soil solution, but long-term effects were not predicted by the model. Compared to harvesting, a higher nutrient release in the soil solution can occur after storms due to root lifting causing increased mineralisation, a larger amount of biomass left at the site due to technical and economic constraints and larger canopy openings. In addition, sea-salt episodes can increase the acidity of the soil solution in the first years after the storm. When considering other ecosystem services, trade-offs can exist between the reduction of nutrient loads in the soil solution and the accumulation of carbon in the forest.

The conclusions drawn from the application of ForSAFE at the forest plot level are valid for the soil water chemistry in the unsaturated zone. In this thesis, an effort has been made to expand the model simulations from the plot to the hillslope scale to understand how forest ecosystems can affect the chemistry of the streams. A new hydrology concept was integrated in ForSAFE-2D that simulates two-dimensional flows of water and chemical elements from the forest to the stream.
ForSAFE-2D allows a better representation of the moisture content by simulating an increasing water saturation level in deeper soil layers and towards the stream. The simulated transport of a tracer along a hillslope shows that the model is capable of capturing the average concentrations of the tracer in the stream. This capability is based on a correct representation of the long-term average runoff and of tracer concentrations in the soil solution.

The results also highlight some of the issues that should be addressed by follow-up research studies. The partitioning of water between base flow and peak flows suggests that the simulation of flow paths by ForSAFE-2D should be re-evaluated. A correct representation of flow paths will be crucial when simulating the transport of elements or compounds which change concentration with depth or distance from the stream (e.g. dissolved organic matter). In addition, the effects of saturation on weathering, as well as decomposition, show that the regulation of these processes at increasing moisture contents should be updated. Finally, the process regulating the allocation of carbon and nutrients to foliage should be revised to increase the share of foliage in the tree biomass and thereby correct the simulation of evapotranspiration.
Sammanfattning

Skogar tillhandahåller en mångfald av produkter och tjänster som allt är kopplade till vattenresurser. Träd behöver vatten för att växa och samtidigt förändrar träds kvalitén och kvantiteten genom avrinning genom modifisering av vatten- och näringsämneskretsloppet. Förståelsen av sambandet mellan skog och vatten är grundläggande för att kunna utvärdera konsekvenserna av naturlig och antropogen påverkan, såsom klimatförändring och skogsbruksåtgärder, på försörjningen av skogsprodukter och tjänster.

På grund av ekosystemens komplexitet används ofta modeller för att förstå interactionerna mellan olika delar av systemen under förändrande förhållanden. ForSAFE är en dynamisk, mekanistisk ekosystemmodell som simulerar lagring och flöde av kemiska ämnen i skogsekosystem. Modellen har utvecklats för att bättre förstå påverkan av miljöförändringar på skogsbiomassans kemi samt mark- och markvattenkemi på skogsbästsandnivå.

De första två studierna i denna avhandling är exempel på tillämpning av ForSAFE i skogsbestånd i södra Sverige. Modellen används för att simulera effekterna av naturliga och antropogena störningar på olika ekosystemindikatorer, inklusive indikatorer för markvattenkvalitet. Studierna visar att näringsämnesurlakning nedanför rotonen är positivt relaterad till näringsämnesrotation på platsen, markstörningar samt mängden organiskt material som lämnats kvar efter avverkning eller storm. Båda störningstyperna leder till en tillfällig ökning av surhetsgraden i markvatten men långsiktiga effekter förutsågs inte av modellen. Jämfört med avverkning kan det förekomma en ökad frigöring av näringsämnen i markvatten i markvatten efter stormar på grund av rotryckning som orsakar ökad mineralisering, en större mängd biomassa som lämnas kvar på plats på grund av tekniska och ekonomiska begränsningar samt större öppningar i krontaket. Dessutom kan havssaltsepisoder öka surhetsgraden av markvatten i de första åren efter stormen. När man beaktar andra ekosystemstjänster kan det behövas avvägningar mellan minskningen av näringsämnesbelastning i markvatten och kollagring i skogen.

De slutsatser som kan dras från användningen av ForSAFE på skogsbästsandnivå gäller för markvattenkemi i den omättade zonen. I denna avhandling har modell simuleringarna utvecklats från beståndsnivå till sluttningsnivå, för att förstå hur skogsekosystem kan påverka kemin i små vattendrag. Ett nytt hydrologiskt koncept har integrerats i ForSAFE-2D, som...
simulerar tvådimensionella flöden av vatten och kemiska ämnen från skogen till vattendraget.

ForSAFE-2D möjliggör en bättre representation av fukthalten genom att simulera en ökad vattenmättnadsnivå i djupare jordskikt och närmre vattendragen. Den simulerade transporten av ett spårämne utmed sluttningen visar att modellen är kapabel att fastställa den genomsnittliga koncentrationen av spårämnet i vattendraget. Denna förmåga är baserad på en korrekt beskrivning av det långsiktiga genomsnittliga flödet och spårämneskoncentrationen i markvattnet.

Resultaten belyser också några frågor som bör behandlas i uppföljningsstudier. Uppdelningen av vatten mellan basflöde och maximalt flöde antyder att simuleringen av flödesvägar i ForSAFE-2D bör utvärderas på nytt. En korrekt beskrivning av flödesvägar kommer att vara nödvändig vid simulering av transporten av grundämnen och föreningar som ändrar koncentration beroende på djup eller avstånd från vattendrag (t.ex. löst organiskt material). Dessutom visar effekterna av mättnad på vittring såväl som på nedbrytning att reglering av dessa processer vid ökande fukthalt bör uppdateras. Slutligen bör processen som reglerar allokeringen av kol och näringsämnen till blad/barr ses över för att öka andelen blad/barr i trädbiomassan, och därmed korrigeras simuleringen av evapotranspiration.
List of Papers


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Author Contributions

I  GZ prepared the model inputs and model parameterization supported by SB, LY and CA. GZ performed the model simulation and data analysis with inputs from LY and SB. CA and SB provided overall guidance throughout the work. GZ wrote the paper with contributions from all authors.

II LY prepared the model inputs and model parameterization supported by GZ, SB and CA. LY performed the model simulation and data analyses with inputs from GVH and GZ. CA and SB provided overall guidance throughout the work. LY wrote the paper with contributions from all authors.

III GZ developed the model concept with the support of SB. LY and HG contributed to a further refinement of the model. KB and SK provided the experimental data used to test the model. CA provided overall guidance throughout the work. All authors contributed to data analysis. GZ wrote the paper with contributions from all authors.

IV GZ developed the model with the support of SB and LY. JO, KB and SK provided model input data or experimental data to test the model. GZ performed the model simulation and data analysis with inputs from LY and SB. GZ wrote the paper with contributions from all authors.

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Acronyms

ANC Acid neutralizing capacity
Bc Base cations, including calcium, potassium and magnesium
BC Base cations, including calcium, potassium, magnesium and sodium
C/N carbon to nitrogen ratio
Ca$^{2+}$ Calcium ion
Cl$^-$ Chloride ion
CO$_2$ Carbon dioxide
DOC Dissolved organic carbon
EMEP European Monitoring and Evaluation Programme
FAO Food and Agriculture Organization of the United Nations
ICP International Co-operative Programme On Assessment and Monitoring of Air Pollution Effects on Forests
K$^+$ Potassium ion
MCPFE Ministerial Conference on the Protection of Forests in Europe
Mg$^{2+}$ Magnesium ion
N Nitrogen
Na$^+$ Sodium ion
NH$_4^+$ Ammonium
NO$_3^-$ Nitrate
N-tot Total nitrogen (nitrate and ammonium)
SO$_4^{2-}$ Sulphate
SWETHRO Swedish Throughfall Monitoring Network
TDR Time Domain Reflectometry
UNECE United Nations Economic Commission for Europe
XRPD X-Ray Powder Diffraction
Introduction

Forests provide multiple products and services (EEA, 2015). The environmental changes to which forests are exposed, natural or human-induced, affect the quantity and quality of the products and services that forests can supply.

The understanding of ecosystem functioning is fundamental to assess the consequences of natural and anthropogenic pressures, such as climate change and forest management, on the provision of ecosystem services. It is through this knowledge that policies and measures aiming to prevent or reduce negative environmental impacts are usually developed.

Research plays a key role in responding to these needs through the analysis of data and the simulation of processes with models. The support of models is often required due to the complexity of the natural ecosystems. They are used to understand the interactions between different system components, the processes regulating fluxes of energy and material and the effects of environmental changes.

All the services provided by forests are linked to water resources, because all biophysical processes are affected by water, i.e. trees need water to grow and, at the same time, they affect the quality and the quantity of soil water and runoff. Policy initiatives have recognized this link and the need of receiving support from science to better understand forest-water interactions. This thesis aims to contribute to a better knowledge on these interactions.

Forest and water policy

A first global consensus on forests was reached at the Earth Summit in 1992 with the statement of the Forest Principles that aimed “to contribute to the management, conservation and sustainable development of forests and to provide for their multiple and complementary functions” (United Nations, 1992). The Principles stress the importance of adopting a holistic view by stating that “all aspects of environmental protection and social and economic development as they relate to forests and forest lands should be integrated and comprehensive”.

Water is among the listed forest services and it is recognized that forests have a “role in protecting … watersheds and freshwater resources” (United Nations,
In the past decades, multiple initiatives have been taken to highlight the importance of the relationships between forests and water.

The Forests and Water Agenda, promoted by FAO, has been key in helping recognize the role of forests in the hydrological cycle (FAO, 2013). In a first phase, it promoted the discussion on forest-water interactions in the context of a changing environment. More recently, it is calling for the development of concrete actions to integrate science, policy and practice regarding forests and water (Figure 1).

FAO’s Five-Year Action Plan is one of the latest activities in the Forests and Water Agenda, and it aims to develop actions to promote the integration of different themes in the period 2016-2020. “Science” is one of the three main themes of the Plan, stressing the need to “promote and intensify international research on forest-water interactions, addressing knowledge gaps”. The theme stresses the importance of increasing the understanding of these interactions when considering climate-change scenarios and different scales. It also recognizes that research studies investigating the relationships between water and forests should better represent different conditions and contexts to avoid “misconceptions and inappropriate management” (FAO, 2015).

In the UNECE region, the Convention on the Protection and Use of Transboundary Watercourses and International Lakes (UNECE Water Convention) was adopted in 1992. It aims at “strengthening transboundary water cooperation and measures for the ecologically sound management and protection of transboundary surface waters and groundwaters”. Although the word forests does not appear in the Convention text, the Convention does make provisions for addressing the effects of human activity on, amongst others, flora, fauna, soil and landscapes. Recently, the Convention recognized the challenges posed by population growth, economic
development, increased energy and food needs on natural resources. The parties decided on the need to carry out assessments of the interlinkage between water, energy, food and ecosystems. The report on the first three water basin case-studies includes assessments of the effects of deforestation, reforestation, forestry and agroforestry (UNECE, 2015).

At the European Union level, the Water Framework Directive (2000/60/EC) has been relevant in promoting the protection and improvement of water resources, but it is weak in addressing the link between water and forests. To help identify anthropogenic pressures on water resources, the Directive requires the collection of information on land use, including forests where relevant. However, there are no further indications on the link between forests and water status nor specific measures to be implemented in the forestry sector (Futter et al., 2011).

Common strategies on forests and water have been promoted by Forest Europe, i.e. the former Ministerial Conference on the Protection of Forests in Europe, as was exemplified in Resolution W2 at the 5th MCPFE in 2007 in Warsaw. With the Resolution, the signatory countries commit to promote sustainable management of forests in relation to water resources, coordinate policies on forests and water, promote actions in the context of forest, water and climate change, and facilitate the economic valuation of water-related forest services.

The role of forests in the water cycle is also advocated by national initiatives. Sweden has identified 16 environmental objectives, eight of which concerning water resources directly. The link with forests and forestry is specifically mentioned in several contexts: the impact on acidification, nutrient leaching causing eutrophication, the achievement of good environmental status in rivers and lakes, possible damages to wetlands and impacts on water resources in forests ecosystems (Naturvårdsverket, 2016).

Water and nutrient interactions in forest ecosystems

Tree growth is dependent both on atmospheric and terrestrial resources. The atmospheric resources include radiation, temperature and CO₂ concentration. The terrestrial resources include water and nutrients which are taken up, retained and released by trees.

Water is necessary for photosynthesis as it is the source of hydrogen to fix carbon in biomass. It is transported from the roots to the leaves following the difference of water potential between soil and atmosphere (Cowan, 1965). The water that is not used for photosynthesis is released back to the atmosphere through transpiration. Besides being a resource for trees, water is also a medium for nutrient transport and it affects nutrient cycling.
Nutrient cycling determines the amount of nutrients that are available for plant growth. It involves the transfer of nutrients into and out of the ecosystem as well as within the ecosystem (Likens et al., 1981; Perry et al., 2008). All the main processes involved in nutrient cycling are affected by moisture content in the soil. At the same time, nutrients influence the availability and the quality of water resources.

Nutrients enter the biochemical cycle in local ecosystems through atmospheric deposition, mineral weathering and biological fixation (Perry et al., 2008).

Water plays a fundamental role in transporting nutrients from the atmosphere to the biosphere through deposition of chemical elements contained in rain and water vapour. This type of deposition is classified as wet deposition. Together with dry deposition – particles deposited by wind – it determines the total nutrient input from the atmosphere. A study comparing throughfall (representing total deposition) and bulk deposition (representing wet-only deposition) of sulphate in forest sites in Europe shows that wet deposition is the largest component of atmospheric input (Lorenz and Granke, 2009). The study shows that wet deposition of sulphate in 2000-2005 was about 78% of the total deposition.

Mineral weathering happens mainly by contact between rocks and water. Water contributes to increase the weathering rates by physical or chemical actions (Blume et al., 2010; Jackson and Sherman, 1953). Water increases the exposed mineral surfaces by breaking rocks through freeze-thaw action and through abrasion (physical weathering). Water is also the solvent necessary to produce chemical weathering.

Biological nitrogen fixation in the soil increases with moisture content (Cusack et al., 2009; Srivastava and Ambasht, 1994). However, at high moisture contents, nitrogen fixation can be inhibited due to the reduced availability of oxygen and carbon dioxide and lower soil temperature (Dixon and Wheeler, 1983). Nutrients are lost from local ecosystems as dissolved substances, solid particles or gases. Water is the carrier for both solutes and part of the solid particles. The greater the magnitude of the runoff in the system, the greater the loss of nutrients. The export as solid particles can play an important role in steep and exposed soils. Nutrients are lost as solutes mainly in forests with oversaturated or acidified soils (Perry et al., 2008).

Once the nutrients are taken up by plants, they tend to cycle within the ecosystem. This nutrient recycling has been described as the intrasystem nutrient cycle which is denoted by the transfer of nutrients among dead and living biomass pools (Perry et al., 2008). Water is essential to the intrasystem cycle because nutrients are absorbed by living organism mainly from the soil solution and they are released back to the soil solution through decomposition. However, the effect of moisture on decomposition rates is still uncertain. For instance, some studies found that decomposition increases linearly with precipitation (Zhang et al., 2008); other studies found that respiration is maximized within a certain moisture range and decreases towards extreme moisture contents (Tang and Baldocchi, 2005); in other
cases, no clear relationship is found between decomposition rates and moisture (Xiao et al., 2014). Likewise, the uptake of nutrients by plants is only partially dependent on water availability. The nutrients must be dissolved in water to be absorbed by trees. However, the transport within plant cells is not fully coupled with water transport, since nutrients can be absorbed through passive and active mechanisms (Mitra, 2015) that allow nutrient absorption also in dry conditions.

As stated earlier in this section, nutrients can also affect the quality and quantity of water resources. The availability of nutrients influences plant growth and thereby water consumption. As a consequence, the water pool in the soil and runoff change. In addition, high nutrient concentrations can reduce the quality of water and lead to eutrophication of stream and lakes and eventually to high nutrient loads to coastal waters. A well-known effect of high nutrient loads is the increasing trend of hypoxia in the Baltic Sea, i.e. the decrease of oxygen concentrations in the water compromising the functioning of the aquatic ecosystem (Carstensen et al., 2014; Conley et al., 2011).

Forest biogeochemical models

Due to the complexity of natural ecosystems, models are often required to understand the processes regulating the system. The modelling of environmental systems can be based on different approaches. Starting from simpler to more complex approaches, models can be defined as empirical, conceptual or process-based (Letcher and Jakeman, 2010). Empirical models simulate ecosystem responses based on the analysis of observations. Conceptual models are based on a simplified representation of processes regulating the system and the model parameters usually do not have a physical or biological meaning. Processed-based models are based on equations that provide a physical explanation to the system processes.

Biogeochemical models simulate the ecosystem processes as transfer of chemical elements between biological and physical system components (Hellweger, 2008). The simulation of processes is usually process-based, but it can be integrated with conceptual or empirical model components when the principles regulating the process are not fully understood.

There is a wide range of biogeochemical models applied to forest ecosystems at different spatial and temporal scales (Homann et al., 2000; Tikta and van Grinsven, 1995; Waring and Running, 2007). They all include a hydrological component that usually simulates deep percolation and surface runoff at the level of the modelled spatial unit (e.g. forest plot, grid cell). However, these models are originally built to simulate independently each ecosystem unit and do not include the lateral water and chemical transport across the units (Naden et al., 2000). More
recently, studies that propose improved hydrological concepts within these models (Machimura et al., 2016; Tang et al., 2014) or the coupling with hydrology models simulating subsurface flows (Katsuyama et al., 2009; Lessels et al., 2015) are emerging. However, there is still a need for the application of mechanistic approaches at different spatial and temporal scales to be able to understand the dynamics of water and nutrient transport from forest ecosystems under a changing environment. Different approaches can address different questions and provide general conclusions useful for policy making.

Aims and objectives

The main aim of this thesis is to provide a method to simulate the nutrient transport from forest ecosystems to surface waters under changing environmental conditions and apply it to boreal forests in Sweden. The biogeochemical model ForSAFE (Belyazid et al., 2006; Wallman et al., 2005) is used for this purpose.

The main research aim is achieved by:

- Evaluating the capability of the model ForSAFE to simulate soil water chemistry in boreal forest ecosystems. The model is evaluated through the comparison with long-term measurements collected in monitored forest sites in Sweden (Paper I-II).
- Investigating the effect of environmental changes on the water resources in forest ecosystems through the application of the model ForSAFE under different disturbance scenarios (Paper I-II).
- Developing a two-dimensional soil hydrological model concept, including lateral water flow and a saturated zone, compatible with the structure of the ForSAFE model and testing it against measurements (Paper III).
- Integrating the two-dimensional hydrological model into the ForSAFE model, and evaluating the capability of the endorsed model to simulate water and chemical flows to the stream. The evaluation is based on the simulation of water flows and the transport of chloride along a forest transect in Northern Sweden and the comparison to measurements in the stream (Paper IV).
Materials and Methods

Study sites

The research presented in this thesis includes studies at the forest site level (Papers I-II) and on a forest transect (Papers III-IV). The first two studies were carried out on forest sites from the SWETHRO and ICP networks. The second two studies produced model simulations along the S-transect in the Krycklan catchment, in Northern Sweden.

SWETHRO and ICP networks (Papers I-II)

The Swedish Throughfall Monitoring Network (SWETHRO) is a unique monitoring network of Swedish forests (Pihl Karlsson et al., 2011). It includes 64 forest sites (2016) across the entire country, in which data on deposition and soil water chemistry are collected. The length of the data series is variable, stretching back up to 30 years for the initial sites that were established in 1985.

The SWETHRO sites are often in forest areas included in the Level II of ICP forests, i.e. forest sites part of the International Co-operative Programme on Assessment and Monitoring of Air Pollution Effects on Forests operating under the UNECE Convention on Long-range Transboundary Air Pollution. The ICP network provides data on tree biomass, soil chemistry and other parameters such as foliage chemistry and defoliation (Figure 2).

The studies presented in this thesis are conducted in two sites in Southern Sweden: Västra Torup (56.14 N, 13.51 E) and Klintaskogen (55.62 N, 13.44 E). The sites belong both to the SWETHRO and ICP network and they are both managed spruce forests. More detailed information on the two sites are reported in Papers I and II.
Figure 2 – SWETHRO and ICP sites
Map representing the location of the SWETHRO and ICP sites in Sweden. The picture on the left show the collectors for throughfall deposition in the SWETHRO forests (photo by Giuliana Zanchi).

Measurements
Data collected in Västra Torup and Klintaskogen are used in three ways: a first set serves as input data to the model, a second set to calibrate organic nitrogen retention and to backcast historical base saturation and a last set is to evaluate the simulation of forest growth and of the soil water chemistry at the forest site level (Papers I and II) (Table 1).
Table 1 - Measurements from the study sites
Measurements used as input data, to calibrate the model and to evaluate the modelled soil water chemistry at the site level.

<table>
<thead>
<tr>
<th>Measurement type</th>
<th>Use</th>
<th>Paper</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soil profile</td>
<td>Model input&lt;br&gt;Data from a soil profile are used to determine the soil structure in the model which is a column divided in homogeneous soil layers.</td>
<td>I-II</td>
</tr>
<tr>
<td>Grain size distribution</td>
<td>Model input&lt;br&gt;Used to determine parameters of the simulated soil column, such as the hydraulic properties and densities of the soil.</td>
<td>I-II</td>
</tr>
<tr>
<td>Soil chemistry</td>
<td>Model calibration&lt;br&gt;The C/N ratio in the soil organic matter is used to calibrate the organic nitrogen retention.&lt;br&gt;In addition, data on current base saturation are used to backcasting of historical base saturation.&lt;br&gt;Model input&lt;br&gt;Data on soil chemistry are used to determine soil parameters (e.g. cation exchange capacity) used as model inputs.</td>
<td>I-II</td>
</tr>
<tr>
<td>Total elemental composition</td>
<td>Model input&lt;br&gt;The total elemental composition is used to determine the mineral composition of the simulated soil column with the model A2M (Posch and Kurz, 2007).</td>
<td>I-II</td>
</tr>
<tr>
<td>Deposition</td>
<td>Model input&lt;br&gt;Open field and throughfall data are used to downscale the modelled EMEP deposition (sulphur and nitrogen) and estimate deposition of base cations, chloride and sodium.</td>
<td>I-II</td>
</tr>
<tr>
<td>Management /Disturbance</td>
<td>Model input&lt;br&gt;Information from management plans and records on natural disturbances are used to determine the management scenarios that simulates the biomass losses at the site due to natural or anthropic disturbances.</td>
<td>I-II</td>
</tr>
<tr>
<td>Forest inventory data</td>
<td>Model evaluation&lt;br&gt;The modelled biomass is compared to the biomass estimated with inventory data to evaluate the simulated forest growth under the past and current environmental conditions, including management and disturbances.</td>
<td>I-II</td>
</tr>
<tr>
<td>Soil water chemistry</td>
<td>Model evaluation&lt;br&gt;Samples of the soil solution collected at 50 cm depth with tension cup lysimeters are used to evaluate the simulation of the soil water chemistry at the forest site.</td>
<td>I-II</td>
</tr>
</tbody>
</table>

The S-transect (Papers III-IV)

The long-term monitored hillslope denoted as S-transect is located in the Krycklan catchment in Northern Sweden (64°14’N 19°46’E) (Figure 3). Krycklan is an experimental catchment of about 68 km², unique for the amount of data collected and the length of the data series (Laudon et al., 2013). The S-transect is located in the Västrabäcken sub-catchment which is forest dominated. The main tree species in the lower part of the catchment is Norway spruce which is gradually substituted
by Scots pine towards the water divide. The transect is aligned parallel to water flows towards the Västrabäcken stream.

Three monitoring points have been established since 1995 along the transect at 4, 12 and 22 m from the stream (S4, S12, S22). Long-term data series of soil moisture, soil water chemistry and groundwater level are available from these profiles (Laudon et al., 2013). Starting from 2013, groundwater level data are available from a well close to the water divide. A sampling point, denoted as C2, was also established in the Västrabäcken stream in 1986, collecting information on streamflow and water chemistry.

Additional data collected in the area include soil mineralogy and grain size distribution, hydraulic properties, geological information, atmospheric deposition, climate data and vegetation data.

Figure 3 – The S-transect in the Krycklan catchment
Illustration of the S-transect and its location in the Krycklan catchment and in Sweden. Measurements of soil moisture, water chemistry and groundwater level from 4 points along the transect (S4, S12, S22, WD) are used in this thesis.
Measurements

Measurements collected along the transect and in the nearest sampled stream (C2) are used as input data to the model, to calibrate or evaluate the simulation of the hydrology and the transport of chemical elements on a forest slope (Paper III-IV) (Table 2).

<table>
<thead>
<tr>
<th>Measurement type</th>
<th>Use</th>
<th>Paper</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grain size distribution</td>
<td>Model input Samples from 6 points along the transect are used to determine the soil texture of the simulated soil columns.</td>
<td>III-IV</td>
</tr>
<tr>
<td>Soil mineralogy (XRPD method)</td>
<td>Model input Samples from 5 points along the transect are used to determine the mineral composition of the simulated soil columns.</td>
<td>IV</td>
</tr>
<tr>
<td>Climate</td>
<td>Model input Precipitation and temperature data at the site are used as climate inputs when available.</td>
<td>III-IV</td>
</tr>
<tr>
<td>Deposition</td>
<td>Model input Measurements of bulk precipitation and throughfall are used as model inputs.</td>
<td>IV</td>
</tr>
<tr>
<td>Soil hydraulic properties</td>
<td>Model evaluation Evaluation of the pedotransfer functions used in the model to calculate the soil hydraulic properties.</td>
<td>III</td>
</tr>
<tr>
<td>Tree inventory data</td>
<td>Model calibration Tree diameters are used to assess tree biomass, compare it to the modelled biomass growth and calibrate vegetation model parameters.</td>
<td>IV</td>
</tr>
<tr>
<td>Soil moisture (TDR)</td>
<td>Model calibration or evaluation Modelled soil moisture is compared to measurements for calibration of the percolation at the bottom of the soil columns (III) or evaluation of the modelled soil moisture (IV).</td>
<td>III-IV</td>
</tr>
<tr>
<td>Ground water level</td>
<td>Model calibration The ground water level data are used to calibrate the percolation at the bottom of the soil columns.</td>
<td>IV</td>
</tr>
<tr>
<td>Streamflow</td>
<td>Model evaluation Information on daily runoff are used to evaluate the modelled streamflow.</td>
<td>III-IV</td>
</tr>
<tr>
<td>Soil water chemistry: chloride concentration</td>
<td>Model evaluation Modelled soil water chemistry is evaluated against measurements.</td>
<td>IV</td>
</tr>
<tr>
<td>Chloride concentration in the stream</td>
<td>Model evaluation Modelled stream water chemistry is evaluated against measurements.</td>
<td>IV</td>
</tr>
</tbody>
</table>
The ForSAFE model

ForSAFE is a dynamic, mechanistic ecosystem model simulating the storage and fluxes of chemical elements in forest ecosystems. It was developed to better understand the effects of environmental changes on the chemistry of forest biomass, soil and soil water (Belyazid et al., 2006; Gaudio et al., 2015; Wallman et al., 2005) (Papers I-II). The model can simulate the effect of changes in climate, management and deposition. The chemical elements included in the model are: nutrients necessary for tree growth (nitrogen, base cations) and chemical elements affecting or affected by the acidity of the soil and water (chloride, sulphur, sodium, dissolved organic carbon (DOC) and aluminium).

Based on canopy size, foliar nitrogen content, temperature conditions and solar radiation, the model simulates the potential vegetation growth at the site which is translated into a water and nutrient demand. The potential growth is constrained to actual biomass growth by water and nutrient availability in the soil and disturbances (Figure 4).

Figure 4 – The ForSAFE model
The figure represents the main drivers of vegetation growth in the ForSAFE model. The potential tree growth is driven by temperature and solar radiation. This potential growth is constrained by water and nutrient availability. Nutrient availability is determined by decomposition, deposition and mineral weathering. Tree growth is further affected by disturbances.
Nutrient availability is given by the nutrient concentrations in the soil solution. This concentration is the result of different processes: atmospheric deposition, hydrological transport, decomposition of organic matter, mineral weathering, adsorption and desorption in the soil and plant uptake.

Water availability is given by the soil water content above wilting point at each time step. The soil moisture is the result of water flows in and out the soil profile. At a given time-step, the moisture is calculated as the balance between water inputs (infiltration) and outputs (evapotranspiration, percolation).

Plant growth influences the nutrients and water directly and indirectly. The direct effects are the nutrients and water uptake by plants that reduce their availability in the soil. The trees also affect water and nutrient resources indirectly by producing organic matter that modifies the soil solution through the release of DOC and is a source of nutrients when decomposed.

Input data to the model include climate, deposition, management, soil and vegetation data (Table 3).

<table>
<thead>
<tr>
<th>Input</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Climate</td>
<td>Long term climate series for the simulation period including mean, maximum and minimum temperature, precipitation, radiation, atmospheric CO₂ concentration. The series include future climate projections to 2100. The data are the results from the interpolation of historical data and climate models’ simulations (ECHAM5, CCSM3, STRÅNG) scaled or substituted by measurements when available. Climate data determine the time step of the model calculations and are on a monthly (Papers I-II) or daily basis (Paper IV).</td>
</tr>
<tr>
<td>Deposition</td>
<td>Annual atmospheric deposition of sulphate (SO₄²⁻), nitrate (NO₃⁻), ammonium (NH₄⁺), base cations (Ca²⁺, K⁺, Mg²⁺), chloride (Cl⁻) and sodium (Na⁺) for the entire simulation period, up to 2100. The data for SO₄²⁻, NO₃⁻ and NH₄⁺ are the results of the simulation with deposition models (MATCH, EMEP). The remaining deposition data are calculated from measurements of bulk precipitation and throughfall deposition.</td>
</tr>
<tr>
<td>Management / Disturbance</td>
<td>Management scenarios describe the biomass losses due to harvesting and natural disturbances. They are based on historical records on forest management and natural disturbances, as well as on information from managers and management plans.</td>
</tr>
<tr>
<td>Soil</td>
<td>The simulated soil columns are structured as different soil layers with homogeneous properties corresponding to the observed soil profiles at the site. These properties include: number of layers, individual layer depth, grain size distribution, organic matter content, base saturation, cation exchange capacity, root fraction, bulk density (when available) and mineral composition. The mineral composition can be derived from the total elemental composition of the soil (Papers I-II) or from measurements (Paper IV). The grain size distribution (alt. texture) is also used to calculate other soil parameters used as inputs, such as the exposed mineral surface, bulk density (when missing) and the hydraulic soil properties.</td>
</tr>
<tr>
<td>Vegetation</td>
<td>The dominant tree type is specified to simulate biomass growth, nutrient and water uptake and litterfall by the vegetation. A set of vegetation parameters is used to describe a given tree type based on previous research studies.</td>
</tr>
</tbody>
</table>
FORSAFE-2D: developments of the hydrology concept (Papers III-IV)

In the original ForSAFE, water fluxes through the ecosystem included only the vertical flows of precipitation, percolation and evapotranspiration, with the assumption that soil is free-draining (Belyazid, 2006; Lindström and Gardelin, 1992). This concept was designed for simulations at the forest site level, where a single homogeneous forest unit is considered. In this thesis, the hydrology of ForSAFE was modified to include lateral water flows which allows water and chemical elements to flow between different forest units and to the stream. The new hydrology also entails a distinction between the saturated and unsaturated zone in the soil and creates a connection to the streams.

By including the endorsed hydrology in ForSAFE, the 1-dimensional fluxes of water and chemical elements become 2-dimensional. Therefore, in the following sections, the updated version of the model is named ForSAFE-2D to distinguish it from the original version of the model. In ForSAFE-2D, the forest is represented as a series of homogeneous forest plots, aligned from the water divide to the stream. Water and chemical elements are transferred from one plot to the other through lateral flows. Each plot has the same structure as in ForSAFE: a soil column divided in different soil layers and covered by vegetation.

Starting from the original hydrology module based on the model PULSE (Lindström and Gardelin, 1992), the new hydrology concept introduces three breaks that constrain the movement of water in the soil and produce soil saturation and lateral water flows (Paper III).

1. The water flow from a given soil layer is constrained by the amount of water that receiving layers can accept vertically and horizontally. This break is determined by the calculated soil porosity and moisture content of the receiving layer.
2. The water flow is regulated by the soil conductivity that controls the amount of water that can move within each time step. The conductivity is calculated based on the soil texture and the simulated soil moisture.
3. The percolation from the bottom of the soil column is constrained to account for the low permeability of deep soil layers. This break is calibrated based on the measured base flow at the site.

Figure 5 illustrates the hydrology concept with a Causal Loop Diagram (CLD). In a CLD, an arrow denotes a causality, indicating that the variables at the origin of the arrow controls the variable at its end. The type of relationship between the two variables is explained by the sign given to the connection: a positive sign indicates that the variables change in the same direction, a negative sign that they change in opposite directions. For instance, an increase of soil moisture results in a higher percolation from the soil layer (+). However, the higher the percolation, the lower the moisture in the soil layer (−).
Precipitation is divided into rain and snow though a snow routine based on air temperature. The snow routine is the same as in the original ForSAFE (Belyazid, 2006). The infiltrating water is a sum of rain and water melting from the snow pack and it is constrained by the receiving capacity of the first soil layer. The water that cannot infiltrate is transferred to the next forest plot as surface flow.

Water flows in the soil are first determined by the soil moisture content in the soil layer and by the soil properties (Soil moisture, Soil permeability and Slope). The water that can flow is the excess soil moisture above field capacity. The actual flow is determined by the receiving capacity of the layer below (Percolation) or the adjacent layer in the next soil column downhill (Lateral flow). The lateral flow from the last forest plot downhill and the bottom percolation from all the plots contribute to the streamflow.

Water frost in the soil and upwards water flows due to capillarity draw are not considered in the model.
A detailed description of the equations that regulate water flows in the soil is given in Paper III.

Soil moisture is regulated also by evapotranspiration (ET m³·m⁻²·d⁻¹). In ForSAFE-2D the ET is dynamically calculated and it is driven by canopy interception, photosynthesis and water availability in the soil (Paper IV). ET is the result of two components: evaporation and transpiration. The evaporation is either calculated as a fraction of the precipitation or as the difference between precipitation and the interception by the tree canopy which is determined by the Leaf Area Index. Transpiration is first calculated as potential transpiration based on the gross photosynthesis and the water use efficiency of the trees. As a second step, the potential transpiration is constrained by the water availability in the soil. The water uptake from each layer is dependent on the root fraction. In addition, if the potential transpiration in one layer cannot be met because of low water availability, this unmet water demand (PotTDf) is added to the potential transpiration in the layer below. In other words, trees can meet their demand for water by absorbing water in deeper layers where they still have roots, when upper soil layers are too dry.

Table 4 – Equations regulating evapotranspiration in ForSAFE-2D

<table>
<thead>
<tr>
<th>Formula</th>
<th>Variables</th>
</tr>
</thead>
</table>
| Evaporation (Evap) | Evap: evaporation (m³·m⁻²·d⁻¹)  
| 1) Evap = P · PrecIntF | P: precipitation (m³·m⁻²·d⁻¹)  
| 2) Evap = MIN(P, MaxInt) | PrecIntF: interception fraction (m²)  
| MaxInt = k · LAI | MaxInt: maximum interception (m³·m⁻²·d⁻¹)  
| P_Ti = P − Evap | k: constant (m²·m⁻²·d⁻¹)  
| Transpiration (T) | LAI: leaf area index (m²)  
| RW_i,j = MIN \left( \max \left( 0, \frac{\text{Moist}_{i,j} - \text{WP}_{i,j}}{\text{LP}_{i,j} - \text{WP}_{i,j}} \right), 1 \right) | Po: potential infiltration (m³·m⁻²·d⁻¹)  
| PotTDf_{i,j} = \begin{cases} 0, & \text{if } i = 1 \\ \max (0, \{\text{PotT} · \text{RF}_{i-1,j} + \text{PotTDf}_{i-1,j}\} − \text{T}_{i-1,j}) & \text{if } i > 1 \end{cases} | RW: relative water content (fraction)  
| T_{i,j} = \min (\text{RW}_{i,j} · (\text{PotT} · \text{RF}_{i,j} + \text{PotTDf}_{i,j}) · (\text{Moist}_{i,j} − \text{WP}_{i,j})) / \text{dt} | i: soil layer  
| | j: soil column  
| | Moist: soil moisture (m³·m⁻²)  
| | WP: wilting point (m³·m⁻²)  
| | LP: limit to transpiration (m³·m⁻²)  
| | PotTDf: deficit of potential transpiration (m³·m⁻²·d⁻¹)  
| | PotT: potential transpiration (m³·m⁻²·d⁻¹)  
| | RF: root fraction  
| | T: transpiration (m³·m⁻²·d⁻¹)  
| | dt: time step (d)  

ForSAFE-2D: chemical transport (Paper IV)

When integrating the new hydrology concept in ForSAFE, it was necessary to modify the algorithms that regulate the chemical concentration in each soil layer.
The chemical concentration in the soil solution at each time step is regulated by a mass balance equation that accounts for the inputs, outputs and accumulation of chemical elements in the soil solution (Belyazid, 2006). The equation was modified to account for the import and export of chemicals through the lateral flows (modified from Belyazid, 2006):

\[
(Q_v^0 \cdot [X]_{c,l-1}) + Q_h^0 \cdot [X]_{c-1,l}) + r_x = \left( Q_v + Q_h + z \cdot \frac{d\theta}{dt} \right) \cdot [X]_{c,l} + z \cdot \theta \cdot \frac{d[X]_{c,l}}{dt}
\]

Where \([X]\) (kmol m\(^{-3}\)) is the concentration of the chemical, \(c\) is the simulated soil column, \(l\) is the simulated soil layer, \(Q_v^0\) and \(Q_h^0\) (m\(^3\) m\(^{-2}\) d\(^{-1}\)) are the vertical and horizontal fluxes of water to the soil layer, \(r_x\) (kmol m\(^{-2}\) d\(^{-1}\)) is the production of the chemical, \(Q_v\) and \(Q_h\) are the vertical and horizontal fluxes of water from the soil layer, \(\theta\) (m\(^3\) m\(^{-3}\)) is the moisture of the soil layer and \(z\) (m) is the layer thickness.

The production term \(r\) includes the net difference between weathering (exclusively for BC, i.e. Ca\(^{2+}\), K\(^+\), Mg\(^{2+}\) and Na\(^+\)), mineralisation and net cation desorption (exclusively for BC) on one hand, and adsorption (exclusively for BC) and uptake on the other.

The chemistry of lateral inflow is calculated by multiplying the lateral water flux entering the soil layer by the concentration of the chemicals in the neighbouring layer in the uphill soil column \((Q_h^0 \cdot [X]_{c-1,l})\). The outputs are calculated by adding the lateral water flow to the water leaving the soil layer. This flow is multiplied by the chemical concentration in the layer \((Q_h \cdot [X]_{c,l})\).

**Water-chemistry interactions**

As in ForSAFE, some biogeochemical processes are influenced by the water content in the soil. The main processes regulated by the water content are:

- **Decomposition** – The moisture content affects the decomposition rates of organic matter in the soil. The rate is regulated by moisture using a modified Langmuir adsorption isotherm that describes the physical adsorption of water to a particulate solid (Wallman et al., 2006; Walse et al., 1998)
- **Weathering** – The weathering of minerals is also dependent on the soil moisture. The total weathering rate of a mineral is linearly dependent on the saturation level in the soil layer (Sverdrup and Warfvinge, 1988).
- **Photosynthesis** – The photosynthesis is limited by water availability in the soil. The potential gross photosynthesis is limited by water availability in the soil. The potential gross photosynthesis is multiplied by the ratio between the actual and the potential evapotranspiration to obtain the actual gross photosynthesis (Aber and Federer, 1992; Belyazid, 2006).
Results and Discussion

Effect of disturbances on soil water chemistry (Papers I-II)

The studies in the two forest sites Västra Torup and Klintaskogen show that soil water chemistry is affected by anthropogenic and natural disturbances. Harvesting and storms at the two sites had consequences both for nutrient leaching and the acidity of the soil solution. In the following sections, the term “disturbance” is used to identify both harvesting and storms.

Nutrient leaching

Nutrient leaching is observed at both sites, but at different levels. While nutrient leaching is observed only after clear cutting at Västra Torup, it peaks after relatively small disturbances at Klintaskogen (5-15% of the standing biomass). By analysing the measurements and model simulations, this difference could be linked to:

- the nitrogen status at the site;
- the amount of plant material left at the site after the disturbance;
- and the effect of storms on soil processes, particularly the mineralisation of organic matter.

The nitrogen (N) status is different in the two forest sites (Figure 6). The amount of N inputs from the atmosphere and the content in the organic material is higher in Klintaskogen, indicating a more nitrogen rich site. The larger availability of N could explain why leaching occurs more easily in Klintaskogen than in Västra Torup. Other studies investigating this link report similar conclusions, while inorganic N deposition alone does not directly explain the levels of N leaching (Akselsson et al., 2010; Hellsten et al., 2015; Lepistö et al., 1995).

The status of base cations is not significantly different between the two sites (Figure 6). The increased concentration of base cations after disturbance is most likely coupled to the increased acidity produced by nitrification and nitrate leaching (Lundell et al., 2001).
The plant material left at the site after disturbance can also play an important role in the release of nutrients in the soil water. The study in Västra Torup simulates nitrogen leaching under different management scenarios. The scenarios consider an increasing amount of biomass extraction, such as harvest residues and additional thinnings. The modelled results suggest that by removing forest residues the cumulative nutrient leaching over a rotation period decreases (Figure 7). This effect results from less organic material decomposing in the forest and releasing nutrients in the soil water. When the management intensification also entails the removal of living trees, i.e. an intensified thinning regime coupled with residue removal, the reduction of nitrogen leaching is less pronounced. By reducing the number of trees, the total plant uptake is lower and more nitrogen is found in soil water compared to the management including residue removal only. In the simulation of tree loss by windthrow in Klintaskogen, it was assumed that part of the residues and all the foliage would remain at the site. Since foliage is more nutrient rich than wood, this assumption has probably contributed to the high concentrations of nutrients in the soil solution after the disturbances.
The storm disturbance at Klintaskogen induced a stimulation of the mineralisation and nitrification processes as reported by other studies (Attiwill and Adams, 1993; Dahlgren and Driscoll, 1994; Legout et al., 2009). This stimulation is explained by a disturbance of the fine roots of the trees, having a priming effect on the decomposition process, and possibly a partial physical oxygenation of the soil from the mechanical disturbance of the tree roots and the shallow soil layers. The stimulation of mineralisation following storm events adds a further cause to nitrogen and base cation leaching, which is not seen after harvesting (Dahlgren and Driscoll, 1994).

Acidification

The two studies in Västra Torup and Klintaskogen show that the disturbances can have various effects on the acidity of the soil solution, depending also on the time-frame considered. Overall, the disturbances at the two sites increase the acidity of the soil solution in the short term, but the model does not predict a long-term effect on it.

After the disturbances the acid neutralizing capacity (ANC), which is an indicator of the acidity of the soil solution (Blume et al., 2010), temporarily decreases. The higher mineralisation rates after felling and windthrow lead to an
increased nitrification that, together with nitrogen leaching, decreases the ANC. The results support the theory that in nitrogen saturated soil and under low acid deposition, the effect of nitrification and nitrogen leaching dominates the acidification process (Aandahl Raastad and Mulder, 1999). Moreover, when management is intensified, the removal of residues leads to a decrease of the base cation pool that can also decrease the acidity of the soil solution. The sea-salt effects that are sometimes associated with storms also modify the ANC. They can contribute temporarily to decrease the acidity by adding chloride to the soil solution.

The study in Klintaskogen confirms that DOC is important in determining the pH of the soil solution, as the latter is significantly negatively correlated to it. However, the model does not reproduce patterns of DOC concentrations comparable to measurements that can explain the relationship between disturbances and DOC and its impacts on acidification.

Trade-offs with carbon stock and sinks

When evaluating the effects of environmental changes on the quality of the soil water, trade-offs with other ecosystem services should be taken into account. The study in Västra Torup shows that trade-offs exist between the leaching of nutrients in the soil water and the carbon stock in the forest. Removing organic material from the site after tree felling, has the effect of reducing the nutrients retained in the forest. As a consequence, whole tree harvesting can reduce the nitrogen leaching compared to current management, but it can also result in a decrease of soil organic carbon. In addition, the reduced nutrient availability in the forest can affect the long-term fertility at the site and possibility affect the productivity of the forest in the future. The relative importance of each effect is very much dependent on the societal priorities and on the site conditions: in less fertile forests it might be more important to maintain nutrient pools rather than reducing the nitrogen loads in soil water and vice versa in nutrient rich areas.

Differences between harvesting and natural disturbances

Some fundamental differences between anthropogenic and natural disturbances might help to explain some of the changes of soil water chemistry at the two sites.

- Windthrow may involve the disturbance of roots that further exposes the soil organic matter to mineralisation, even under the soil surface. This can contribute to the release of more nutrients into the soil solution in the first years after the storm.
• The removal of material after a storm can be technically more difficult and less economical than after harvesting. Therefore, it is possible that more material, especially foliage and branches, is left in the forest to decompose.
• Sea-salt episodes associated with storms temporarily increase the ionic strength of the soil solution (e.g. chloride and sodium). These events can affect acidity in the short term.
• Thinnings can have a more uniform effect on tree cover than natural disturbances. At equivalent amounts of biomass affected, a windthrow can produce a large opening in canopy cover while thinnings are uniformly distributed in the forest. Larger open areas favour the mineralisation of organic matter and a faster release of nutrients in the soil water. However, this factor was not included in the model simulations.

Taken these factors into account, at equivalent amounts of biomass affected, natural disturbances can result in larger nutrient release in the soil solution in the short term than harvesting.

Transport of chemical elements to the stream (Papers III-IV)

The chemical concentration of the water reaching the stream depends on the runoff and the chemical concentrations met along the flow paths. Therefore, the correct simulation of the stream chemistry requires a correct representation of the total streamflow, the flow paths and the change of soil water chemistry with depth and distance from the stream. The following two studies included in the thesis aimed to develop and test a new hydrology concept incorporating lateral water flow and to understand the capability of ForSAFE-2D to simulate chemical transport from a forest hillslope to the stream.

Modelled runoff and flow paths

The new hydrology concept and ForSAFE-2D simulate a total runoff consistent with measurements. However, the model tends to overestimate the runoff, mainly due to a modelled base flow higher than the measured one (Paper III and IV).

The overestimation of runoff is higher in the simulation with ForSAFE-2D (Paper IV) than in the test of the hydrology concept only (Paper III). The difference between the two simulations is attributed to the estimates of evapotranspiration in the two studies: 59% of the precipitation in Paper III against 49% in the last paper. When compared to other approaches, the higher evapotranspiration value seems to be more realistic. In ForSAFE-2D the evapotranspiration is simulated dynamically.
based on the tree water use. The analysis of the biomass shows that the model underestimates the share of foliage in the tree biomass. As a consequence, the modelled transpiration, which is linked to the foliage biomass, is probably underestimated.

When analysing both the streamflow at low and high flow rates, evapotranspiration does not fully explain the mismatch between modelled and measured data. The data analysis suggests that two other factors could contribute to these differences.

On the one hand, the 2-dimensional hydrology does not consider soil water frost. This limitation can contribute to the overestimation of the base flow and, consequently, to underestimated peak flows in spring. In reality, the water is retained in the soil in winter as a frozen pool and quickly released with thaw in spring.

On the other hand, the velocity and the paths of water could be misrepresented by the model. The total simulated runoff is the sum of three components: the percolation at the bottom of the modelled soil columns in the hillslope, the lateral flow from the soil column nearest the stream and the surface flow. The studies presented in this thesis show that the assumption that most strongly affects the modelled hydrology is the parametrization of the first component, the bottom percolation. Since ForSAFE-2D simulates the water storage and flows down to a certain depth, it is necessary to constrain the percolation at the bottom of the soil columns to account for the presence of soil below the modelled depth. Without this constraint, the water is free to percolate, no saturated zone can be created and the lateral flows become close to zero. The stronger the constraint, the higher the saturation of the soil and the water transported as lateral flow and surface runoff.

So far, in ForSAFE-2D, the calibration of the bottom percolation is driven by the simulation of saturated soil layers at a depth comparable to the measured ground water level along the hillslope. When analysing the flow paths of the water to the stream, it is evident that on a yearly basis, the larger component of the streamflow is the bottom percolation (58% of runoff in 2010-2015, Figure 8). Second is the lateral flow from the forest plot closer to the stream (32%). Finally, the surface runoff happens concurrently with high precipitation events, when the soil is more saturated (9% of runoff).

When compared to measurements, there seems to be a delay in the modelled water flows. After thaws or intensive precipitation events there is a sharp increase in all the three components of the runoff. However, the simulated peak flows are well below the measurements (Paper III and IV). In addition, the bottom and lateral flows maintain high values for several days after the peak flow, suggesting a delay in the release of water from the soil, when the water inputs are high.
Variability of chemical concentrations in the soil

As illustrated in the first two studies, the original ForSAFE simulates concentrations of the soil solution in the unsaturated zone that are in agreement with measured concentration below the rooting zone. The simulation at Västra Torup also shows that the chemistry of the soil solution might vary significantly with depth and compound. The concentrations of nitrogen, base cation and DOC simulated by the model decrease significantly with depth, while those of sulphate and chloride are relatively stable, and sodium shows an increase (Figure 9).

When considering a hillslope, the chemistry of the soil solution can vary not only vertically with depth, but also horizontally, due to the change of soil properties and saturation levels from the water divide to the stream.

Measurements and model results taken along the S-transect confirm some of the patterns already simulated in the unsaturated zone. The modelled chloride concentrations in the soil water are almost constant with depth or distance from the stream and consistent with the average measured values (Paper IV). The measured data show a certain variability on a daily basis that is not fully captured by the model. This variability is explained by daily changes in deposition that are not taken into account in the model inputs which are provided yearly.
The simulation of the concentration of other elements and compounds shows that some of the processes in the model need to be re-evaluated in future work. For instance, the modelled sodium (Na) concentrations increase strongly with depth, largely overestimating the measured data. The overestimation of Na concentrations at depths beyond the rooting zone is due to unrealistically high weathering rates in the saturated soil (Figure 10). The soil solution is increasingly enriched in Na as the water flows laterally towards the stream, as seen in the highest simulated concentrations closest to the stream (Figure 10).

In a forest transect, ForSAFE-2D produces an increase of saturation with depth and towards the stream (Figure 11) as indicated by measurements. Saturation affects the modelled decomposition and weathering rates and thereby the production term in the mass balance equation of elements like sodium. Previous applications of ForSAFE considered forest sites in which the water table was below the simulated depth. Therefore, they did not include saturated soil layers (Figure 11) neither highlighted the sharp increase of weathering rates at high moisture content.
Figure 10 – Modelled and measured sodium concentrations [Na] in the soil solution. Measured sodium concentrations at 4, 12 and 22 m from the stream are compared to the modelled concentrations up to 25 m from the stream. The sodium concentrations are represented on a logarithmic scale.
Figure 11 – Water saturation levels in the soil in Västra Torup and Svartberget
Change of saturation with depth in Västra Torup (first graph of the left). The change of saturation along the hillslope in Svartberget is represented through six soil columns at increasing distance from the stream (from left to right).
Streamflow concentrations

The strengths and the weaknesses in modelling water flows and chemical concentrations in the soil are reflected in simulating streamflow concentrations.

The average chloride concentration in the stream is correctly assessed by the model because both the average modelled soil concentrations and the total runoff are comparable to measurements. As for the soil water concentrations, daily fluctuations of chloride concentration in the stream are not reproduced by the model, because the daily variability of deposition causing these fluctuations is not accounted for in the model. In addition, chloride is very uniform with depth and distance from the stream and the runoff concentrations are independent from their origin in the hillslope. Therefore, the contribution of different water flow paths to the stream concentrations cannot be deduced from the transport of chloride.

The evaluation of flow paths requires the analysis of elements or compounds like DOC that vary along the hillslope. A first evaluation of the DOC concentrations in the stream show that they are in the same range of variation as the measurements. However, the concentration patterns of DOC in the stream are not simulated correctly (Figure 12). The reasons behind this limitation are:

- The simulated concentration in the soil solution are underestimated in upper soil layer and overestimated in deep soil layers;
- in the model a large share of DOC is transported through the percolation at the bottom of the simulated soil columns.

Figure 12 – Modelled and measured DOC in the stream
Grey line: simulated DOC concentrations in the stream; black dots: measured concentrations.
In forest areas, the analysis of the measurements shows that DOC in the stream increases proportionally with the runoff: at high-peak flows, the DOC concentrations also peak. Since the DOC concentrations in the soil water are much higher in upper layers and in the riparian zone, the measurements suggest that at high-peak flows the water travels mainly through surface layers and the riparian zone (Laudon et al., 2011). In contrast, 59% of the simulated DOC reaching the stream originate from deeper soil layers.

**Future perspectives**

The work presented in this thesis has highlighted a series of limitations in the ForSAFE-2D model that should be addressed to improve the simulation of the dynamic transport of chemical elements and compounds from the forest to the stream. For this purpose, some of the modelled processes should be revised in future research studies.

**Foliage biomass**

The simulated foliage biomass is significantly lower than the measurements, while the total tree biomass is comparable to experimental data. This fact has consequences for both tree water consumption and the production of litter and organic matter. The results suggest that the processes regulating the allocation of carbon and nutrients to wood and foliage should be revised to correct the proportion of foliage in the total biomass.

Canopy size has a direct effect on canopy interception and the concentrations of the solution entering the soil. In addition, plant transpiration and thereby soil moisture are also affected. In the studies discussed in this thesis, the low foliage biomass results in an underestimation of the total transpiration, which has a major role in the water balance of a hillslope.

The production of litter would also be affected and thereby the amount of nutrients returned to the soil. Foliage is more nitrogen rich than wood and has a faster turnover rate. It can be expected that with higher simulated foliage, the amount of organic matter and nutrients returned to the soil will be also higher.
Weathering and decomposition

The simulation of soil with high saturation level has highlighted that the weathering rates increase unrealistically with the moisture content. Previous studies in the unsaturated zone could not detect this trend.

Currently, the weathering production of base cations (including sodium) is slowed down by the increased concentration of weathering products in the soil solution (Sverdrup and Warfvinge, 1993). Recent research has hypothesized that the retardation of the weathering rates at higher base cation concentrations is weak, i.e. the weathering rates should be lower at high base cation concentrations in the soil solution. In addition, silica concentrations should be included as a factor contributing to the retardation of weathering rates (Sverdrup et al., in prep.; Erlandsson et al., in prep).

Similarly, the decomposition rates and consequently the production of DOC are affected by the saturation level. An evaluation of the effects of increases in moisture on decomposition should be a priority in follow up studies and the basis for a revision of the decomposition process, when needed.

Hydrology

The application of the new hydrology concept highlighted that there is a delay in the release of water to the stream. This is caused by the structure of the soil in the model which is discrete and represented by boxes denoting soil layers with different properties. Each soil box can release only a maximum amount of water at each time step determined by the space that can be filled by water, i.e. its porosity. The daily time step determines that each box can be emptied once a day. A representation of the flow closer to reality would allow the water to travel faster through the soil and reach the stream within a day, especially when the water inputs are high and the hydraulic conductivity of the soil increases. An implication of box hydrological models, as in FORSAFE-2D, is that the minimum number of time steps needed to reach the stream is equal to the number of soil boxes to be crossed along the path. As a consequence, the water entering the system tends to accumulate in the soil for longer periods than in reality, causing the delay in the streamflow and a rise of the groundwater level. The larger the number of soil layers to be crossed and the distance to be travelled, the larger the delay. The time needed to flow vertically is on average shorter than that of lateral flow, because the distance to the stream is shorter and the number of boxes is smaller. For these reasons, when water flows laterally rather than vertically there is a higher rise of the groundwater level along the entire slope.

Future research should consider a less constrained flow of water within the soil, especially when water inputs are high. Two possible solutions could be tested:
the introduction of preferential flows and/or the simulation at smaller time steps when the velocity of the flow is high.

Another process that should be included in the model is the simulation of frost in the soil, which would reduce the base flow in winter and release more water in spring, as indicated by measurements.
Conclusions

The first two studies discussed in this thesis are examples of analysis at the plot scale level using the ecosystem model ForSAFE. This type of studies can support the investigation of the effects of environmental changes on different forest ecosystem indicators in an integrated manner. From the presented studies it is possible to draw the following conclusions on the effect of anthropogenic and natural disturbances on soil water.

- The effect of disturbances on nutrient leaching is influenced by the nutrient status of the site, the amount of organic material left in the forest and soil disturbances. The higher the nutrient inputs and pools in the forest, the material left to decompose and the soil disturbances, the higher the nutrient leaching.
- The disturbances at the two sites produced a temporary increase of the acidity of the soil solution, but long-term effects were not predicted by the model.
- A series of factors can contribute to a different response of forest ecosystems to storms and harvesting, when equal amounts of tree biomass are affected. Root lifting, biomass left at the site due to technical and economic constraints and larger canopy opening can contribute to higher nutrient release in the soil solution after storms. In addition, sea-salt episodes can increase acidity in the first years after the storm.
- Trade-offs exist between the reduction of nutrient loads in the soil solution and the accumulation of carbon in the forest.

The conclusions from the studies at the stand level are limited to the soil solution in the unsaturated zone. This thesis has made a further step to link the effects of environmental changes in the forest to the effects on surface waters, by simulating lateral transport and a saturated zone in the soil.

- The new hydrology concept integrated in ForSAFE-2D allows a better representation of the moisture content in the soil which is one of the elements necessary to correctly simulate the chemistry of the soil solution. The range of simulated moisture reaches saturation in deeper soil layers and towards the stream, as reported by measurements.
- The simulated transport of a tracer along the hillslope shows that the model is capable of capturing the average concentration in the stream. This
capability is based on a correct representation of the average runoff and concentrations of the tracer in the soil solution.

- The application of ForSAFE-2D on a hillslope also highlighted that there is a delay in the water flow through the soil caused by the discrete structure of the model. This delay limits the capability of the model to correctly represent the water flow paths and the partitioning of water between base flow and peak flows. As a consequence, the base flow is overestimated and the peak flows are underestimated. The lack of simulation of soil water frost can also contribute to this misrepresentation of streamflow dynamics.

- A correct modelling of flow paths will be crucial when simulating the transport of elements or compounds which change concentration with depth or distance from the stream (e.g. DOC).

- The model testing showed that some of the processes represented in the model should be re-evaluated in future research studies. The application of ForSAFE-2D on a hillslope, showed that at high saturation levels, weathering is not simulated correctly. Decomposition is also regulated by moisture content and the evaluation of the effects of saturation on decomposition rates should be a priority in follow-up studies. Moreover, the allocation of carbon and nutrients in the model should be revised to increase the share of foliage in the trees. The underestimated foliage results in an underestimated evapotranspiration and an overestimated runoff.
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References


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