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Linking distributed hydrological processes with ecosystem vegetation dynamics and carbon cycling: Modelling studies in a subarctic catchment of northern Sweden

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List of papers

I. Tang, J., Pilesjö, P., Miller, P. A., Persson, A., Yang, Z., Hanna, E. & Callaghan, T. V. (2014), Incorporating topographic indices into dynamic ecosystem modelling using LPJ-GUESS. Ecohydrology, 7: 1147–1162. DOI: 10.1002/eco.1446

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III. Tang, J., Miller, P. A., Persson, A., Olefeldt, D., Pilejsö P., Heliasz M., Jackowicz-Korczynski M., Yang Z., Smith B., Callaghan, T.V. & Christensen, T. R. Carbon budget estimation of a subarctic catchment using a dynamic ecosystem model at high spatial resolution. *Submitted*

IV. Tang, J., Poska, A., Yurova, A., Miller, P. A., Olin, S., Smith B. & Schurgers, G. Modelling dissolved organic carbon export within a dynamic ecosystem model: implementation in a subarctic catchment. *Submitted*

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Linking distributed hydrological processes with ecosystem vegetation dynamics and carbon cycling

Modelling studies in a subarctic catchment of northern Sweden

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Title and subtitle: Linking distributed hydrological processes with ecosystem vegetation dynamics and carbon cycling - Modelling studies in a subarctic catchment of northern Sweden

Abstract

The Arctic and Subarctic regions are of particular importance to the global climate change and are now experiencing a climate warming that is higher than the global average. Around 50% of the global soil carbon is stored in high latitude soils, especially in permafrost and peatland soils. Permafrost thawing, speeding up the decomposition of previously frozen soil carbon, is expected to result in strongly positive feedbacks to global warming. Meanwhile, increased air temperature may strongly impact vegetation growth and distributions in this region. Dynamic ecosystem models are powerful tools to study climate change influences on ecosystem processes and also to quantify ecosystem feedbacks to the atmosphere. However, these models often focus on the vertical transfer of carbon and water between the atmosphere, the land surface vegetation and soils. Therefore, they generally do not consider the horizontal water and soluble carbon flows between the modelled spatial units (grid cells), which could result in an incomplete estimation of water and carbon budgets, especially for climatically sensitive high latitude regions.

In this thesis, we aim to overcome this limitation by implementing spatial topographical indices into a state-of-the-art dynamic ecosystem model, LPJ-GUESS, and to incorporate water and carbon (mainly dissolved organic carbon, DOC) interactions between the grid cells. Modelling approaches and algorithms developed in this thesis were applied to study the subarctic Stordalen catchment, located in northern Sweden, and to explore the potential influence on the model's hydrological and ecological estimations. Extensive sets of observation data were used for model evaluation throughout.

We proposed a distributed hydrological (DH) approach to dynamically simulate water flow from cell to cell within the catchment and compared the hydrological and ecological impacts resulting from different flow routing algorithms. The results indicate an improved accuracy of runoff estimation when using the proposed DH scheme in the Stordalen catchment. They also show that the choice of flow algorithm can have strong impacts on water and carbon flux estimations in this region. Furthermore, a complete estimation of the catchment carbon budget was assessed using our developed model. We found that the catchment is a carbon sink at present and could become a stronger sink in the near future, a result which is, however, very dependent on future atmospheric CO_2 concentrations and methane (CH_4) emissions from the peatlands. Additionally, the model was further extended to dynamically model soil water DOC and the lateral transport of DOC across the landscape. The modelled outputs suggest that DOC production and mineralization largely contribute to DOC fluxes and that wet fen peatland is and will be a hotspot for DOC export.

In conclusion, this thesis demonstrates the feasibility of implementing topographical indices into LPJ-GUESS to describe water flows, and the importance of considering spatial heterogeneity in hydrological conditions when modelling carbon dynamics at high latitudes. Furthermore, the integration of vertical and horizontal carbon fluxes at high spatial resolutions can be used to provide more accurate estimations of a complete carbon budget and can dynamically simulate the fate of different carbon components in response to climate change.

Key words: Carbon cycling, Water cycling, Hydrological modelling, Ecosystem modelling, Subarctic ecosystems, Climate change

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Linking distributed hydrological processes with ecosystem vegetation dynamics and carbon cycling

Modelling studies in a subarctic catchment of northern Sweden

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A doctoral thesis at a university in Sweden is produced either as a monograph or as a collection of papers. In the latter case the introductory part constitutes the formal thesis, which summarizes the accompanying papers already published or manuscripts at various stages (in press, submitted, or in preparation).

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List of contributions

I.   TJ contributed to the design of the study, implemented
        topographical indices in LPJ-GUESS, performed all simulations
        and analysis, and led the writing.

II.   TJ led the design of the study, performed all simulations and
        analysis, and led the writing.

III.   TJ led the design of the study, performed all analysis and
        simulations, contributed to the interpretation of the results, and
        led the writing.

IV.   TJ implemented DOC-related processes in LPJ-GUESS, led the
        design of the study, performed all simulations, participated in
        the analysis, and led the writing.

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In this thesis, we aim to overcome this limitation by implementing spatial topographical indices into a state-of-the-art dynamic ecosystem model, LPJ-GUESS, and to incorporate water and carbon (mainly dissolved organic carbon, DOC) interactions between the grid cells. Modelling approaches and algorithms developed in this thesis were applied to study the subarctic Stordalen catchment, located in northern Sweden, and to explore the potential influence on the model's hydrological and ecological estimations. Extensive sets of observation data were used for model evaluation throughout.

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extended to dynamically model soil water DOC and the lateral transport of DOC across the landscape. The modelled outputs suggest that DOC production and mineralization largely contribute to DOC fluxes and that wet fen peatland is and will be a hotspot for DOC export.

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Sammanfattning

De arktiska och subarktiska regionerna är av särskild betydelse för den globala klimatförändringen, och genomgår nu en klimatuppvärmning som är högre än genomsnittshöjningen på jorden. Omkring 50 % av världens markkol är lagrat i nordliga jordar (på höga latituder), och där främst i permafrost- och torvjordar. Upptiningen av permafrost påskyndar nedbrytningen, och därmed frigöring, av tidigare fryst markkol, vilket förväntas ha kraftiga effekter på den globala uppvärmningen. Samtidigt kan en ökad lufttemperatur påtagligt påverka tillväxt och utbredning av vegetation i dessa regioner. Dynamiska ekosystemmodeller är effektiva verktyg för att studera klimatförändringars påverkan på ekosystemprocesser, inklusive kvantifiering av återkopplingar från olika ekosystem till atmosfären. Dessa modeller fokuserar emellertid främst på det vertikala utbytet av kol och vatten mellan atmosfär, landyta, vegetation och mark. Därför tar de i allmänhet inte hänsyn till de horisontella vatten- och kolflödena som förekommer mellan de modellerade rumsliga enheterna (jmf gridceller i en rasterkarta eller pixlar i en bild). Denna förenkling kan leda till en ofullständig uppskattning av vatten- och kolbudgetar, och då i synnerhet för de klimatkänsliga regionerna på de höga latituderna.

Denna avhandling syftar till att reducera ovan nämnda begränsningar genom att implementera rumsliga topografiska index i den dynamiska ekosystemmodellen LPJ-GUESS, samt att inkorporera interaktioner mellan vatten och kol (huvudsakligen löst organiskt kol, DOC) över ytan (mellan gridcellerna i kartan). De modeller som utvecklats inom denna studie har implementerats i det subarktiska Stordalens avrinningsområde, beläget i norra Sverige. Där har modellernas eventuella inverkan på hydrologiska och ekologiska simuleringar analyserats och dokumenterats. För utvärdering av modellerna har omfattande observationsdata använts.

Vidare föreslås en distribuerad hydrologisk (DH) metod för att dynamiskt simulera vattentransport från cell till cell inom Stordalens avrinningsområde, och jämförande studier av de hydrologiska och ekologiska effekterna beroende på olika algoritmer för modellering av vattenflöden har genomförts. Resultaten visar att den föreslagna DH-metoden kan modellera avrinningen i Stordalens avrinningsområde bättre än tidigare föreslagna metoder. Vidare kan det konstateras att valet av flödesalgoritm har en stor inverkan på modelleringen av vatten- och kolflöden i regionen. Den utvecklade metoden användes även för att

utföra en fullständig uppskattning av kolbudgeten i avrinningsområdet. I denna delstudie kom det fram att upptagningsområdet idag är en kolsänka, och att det inom en snar framtid sannolikt kommer att bli en ännu starkare sänka. Detta förlopp är emellertid starkt beroende av framtida atmosfäriska CO_2-koncentrationer och metanutsläpp från torvmarkerna. Den sista delen av avhandlingen behandlar ytterligare utveckling av modellen för att dynamiskt kunna modellera DOC i markvatten, samt den laterala (horisontella) transporten av DOC i landskapet. Resultaten visar att produktion och mineralisering av DOC i stor utsträckning bidrar till DOC-flöden, samt att våta torvmarker är och kommer att vara hetfläckar (även kallade hotspots) för DOC-export.

Sammanfattningsvis visar denna avhandling möjligheterna att implementera topografiska index och vattenflöden (lateralt och vertikalt) i LPJ-GUESS. Den demonstrerar också vikten av att ta hänsyn till rumslig heterogenitet i hydrologiska förhållanden vid modellering av koldynamik på höga latituder. Avhandlingsarbetet har gjort det möjligt att genom integrering av vertikala och laterala kolflöden vid höga rumsliga upplösningar noggrannare skatta en fullständig kolbudget, samt att dynamiskt simulera vilken påverkan klimatförändringarna har på olika kolkomponenter.

摘要

北极和亚北极地区对全球气候变化影响尤为重要。目前，北极地区正面临着变暖速度高于全球平均的现状。全球大约有 50%的土壤碳储存在高纬度地区的土壤里，这些土壤碳主要分布于冻土层和泥炭层中。冻土层的解冻会使原先被冻结的土壤碳加速分解，产生温室气体，从而对全球变暖形成一个强烈的正反馈。与此同时，气温的增加可能会很大程度地影响植被在这些地区的生长和分布。动态生态系统模型是一种非常强大的工具，被用来研究气候变化对生态系统的影响，并且可以量化生态系统对大气的反馈信息。然而这些模型通常只关注大气、地表植被和土壤之间的水和碳的纵向转移，从而忽略了其在模型空间单元中的横向移动。这样可能会导致模型对于水和碳平衡的计算不够准确和全面，尤其在气候敏感的高纬度极地地区，这种偏差可能会更大。

本论文旨在解决动态生态系统模型中的这个局限性问题。基于目前最先进的动态生态系统模型 LPJ-GUESS，我们利用和结合空间地形指数实现了模拟水和碳（主要是土壤溶解性有机碳）在空间单元中的相互作用。文中所提出来的建模方法和算法被应用到坐落于亚北极地区，瑞典北部的 Stordalen 流域，以探索模型新方法对估算水文和生态过程的潜在影响。在整个应用过程中，我们采用了大量的观测数据集来进行模型评估。

我们提出了一种基于网格单元对网格单元的分布式水文（DH）方法来动态模拟流域内的水流。我们进一步比较了不同的流量路径算法对于模拟水文和生态过程的影响。结果表明，当我们在 Stordalen 流域内使用结合了分布式水文方法的模型时，该模型对于径流估算的精度比以往有所提高。同时实验结果也表明了流量路径算法的选择会对研究区域内水通量和碳通量的估算产生重大的影响。基于以上结果，我们（在高空间分辨率下）利用该模型对流域内的碳预算有了一个更为完整的估算。我们发现，Stordalen 流域现在是一个碳汇，并且在不久的将来有可能成为一个更大的碳汇。然而这一预测结果非常地依赖于空气中二氧化碳浓度的增加对流域内植被固碳能力的影响，同时还受流域内泥炭地里甲烷的排放量的影响。除此之外，该模型进一步扩展了对土壤水中的溶解性有机碳（DOC）的含量及其空间横向传输的动态模拟。模拟的输出表明，土壤中 DOC 的动态变化主要受 DOC 的产生量和矿化作用的影响，潮湿的沼泽泥炭地在现在和将来都会是土壤 DOC 输出的热点区域。

总而言之，本论文展示了在 LPJ-GUESS 模型中加入用以描述水流的地形指数的可行性，同时证明了在高纬度地区模拟碳动态变化时对于水文条件的空间异质性的考量的重要性。此外，本论文还说明了在高空间分辨率下，综合考虑垂直和水平碳通量可以提供更准确和更完整的碳预算的估计，也可以动态地模拟不同的碳成分在应对气候变化时产生的不同结果。

Everything should be made as simple as possible, but not simpler

-----A. Einstein

Contents

Abbreviations

$C_{CH4:}$ Potential carbon pool for methanogens
DA: Drainage Area
DEM: Digital Elevation Model
DH: Distributed Hydrology
DOC: Dissolved Organic Carbon
DGVM: Dynamic Global Vegetation Model
fSOC: Fast (i.e. with a high turnover rate) Soil Organic Carbon
GCM: General Circulation Model
GPP: Gross Primary Productivity
LPJ-GUESS: Lund-Potsdam-Jena General Ecosystem Simulator
MF: Multiple Flow
NEE: Net Ecosystem Exchange
NPP: Net Primary Productivity
PFTs: Plant Functional Types
RCM: Regional Climate Model
R_a: autotrophic Respiration
R_{exud}: Root exudates
$R_{h:}$ heteotrophic Respiration
S: Slope
SF: Single Flow
SPSOC: Sorbed Potential Soluble Organic Carbon
sSOC: slow (i.e. with a low turnover rate) Soil Organic Carbon
TWI: Topographical Wetness Index
TFM: Triangular Form-based Multiple flow
WHyMe: Wetland Hydrology and Methane
WTP: Water Table Position

1. Introduction

1.1. High latitude climate change

Since the 1980s, the observed mean annual air temperature in the Arctic/Subarctic region has increased twice as much as in the rest of the world (AMAP, 2012). Warming can accelerate shrinkage of sea ice cover, permafrost (ground that is frozen for at least two consecutive years) thawing, glacier retreat and reduction in snow-cover duration as well as extent (IPCC, 2013). Earlier melting of ice and snow results in more radiation being absorbed by soil, vegetation and ocean surfaces which could in turn increase air temperatures and cause yet more snow and ice melting (Snyder, 2013). Stronger winter warming, relative to summer warming, has been observed (Shindell *et al.*, 1999, AMAP, 2012), which has prolonged the growing season in the Arctic/Subarctic region (IPCC, 2013). This was further supported by Xu *et al.* (2013) who analysed satellite data between 1982 and 2012 and found that around one-third of the Arctic/Subarctic biosphere has greened over the period. Long-term ground-observations have also found that trees and tall shrubs have started to shift upward to higher elevations and poleward to higher latitudes in response to the warming (Shiyatov *et al.*, 2007, Rundqvist *et al.*, 2011, Callaghan *et al.*, 2013). From a carbon cycle perspective, a greener Arctic will likely sequester more carbon, which will have a negative feedback (cooling) on the atmospheric warming. However, this feedback is accompanied by positive feedbacks (warming) resulting from the reduced albedo of the greener land surface (Snyder, 2013) and taller vegetation especially in snow-covered seasons (Miller & Smith, 2012, Zhang *et al.*, 2013).

In high latitudes, annual precipitation has increased by 5% since the 1950s (AMAP, 2012) but has shown large inter-annual variability. Generally, global climate models predict an increase in annual precipitation through the 21st century under all scenarios (Kattsov *et al.*, 2007, Solomon *et al.*, 2009, IPCC, 2013). Winter and spring precipitation are expected to increase most (Kattsov *et al.*, 2007, AMAP, 2012) and could be accompanied by more frequent rain events and mid-winter melting (Burn *et al.*, 2004). Snowmelt normally produces the highest runoff through a year. Warmer winters are likely to shorten the duration of snow-cover (Euskirchen *et al.*, 2007), reduce intensive snowfall and increase rain-on-snow events (Woo, 2012). The peak in runoff during the snowmelt season is likely to

decrease but the winter baseflow (deep groundwater flow) may increase (St. Jacques & Sauchyn, 2009). However, these changes depend on the magnitude of permafrost thaw and the amount of snowfall and rain during the winter. In addition, an earlier snowmelt could lead to an earlier ice break-up in rivers and lakes, due to direct heat inputs from runoff as well as the subsequent reduction in albedo.

1.2. Permafrost and peatland carbon cycling

1.2.1. Permafrost

Around 50% of the global soil organic carbon (SOC) is stored in high latitude soils (Tarnocai *et al.*, 2009), especially in permafrost and peatland soils. The organic carbon stored in high latitude soils is approximately twice the size of all the carbon stored in the Earth's atmosphere(AMAP, 2012, IPCC, 2013). With a temperature increase and the subsequent permafrost thawing in this region, a substantial amount of the stored ('old') organic carbon in high latitude soils could be released to the atmosphere (Zimov *et al.*, 2006, Schuur *et al.*, 2009) (Fig. 1). These processes can provide strong positive feedbacks to climate change (Koven *et al.*, 2011). Another important consideration is that methane (CH_4) production and release becomes a more common pathway of carbon loss with continuous permafrost thaw (Zimov *et al.*, 2006). As CH_4 is a much stronger heat-trapping greenhouse gas than carbon dioxide (CO_2), the release from wet permafrost regions (e.g. thermokarst lakes) can substantially contribute to regional and global climate change (IPCC, 2013).
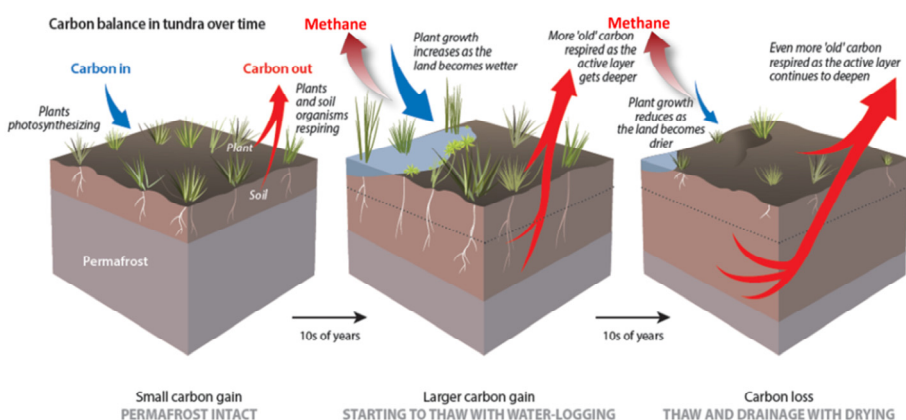

Figure 1. Tundra soil carbon balance in a changing climate (Modified from the source: AMAP (2012)).

2

1.2.2. Northern peatland

Around 50% of the global wetlands are located in high latitudes (Aselmann & Crutzen, 1989, Avis *et al.*, 2011). Peatlands are permanent inundated wetlands where organic matter (peat) has accumulated under waterlogged conditions (Wania, 2007). Generally, northern peatlands exist where the annual temperature is between -12°C to 5°C and annual precipitation is between 200 mm and 1000 mm (Yu, 2012). Peatland soils contain one-third of the global soil carbon (Gorham, 1991, Roulet *et al.*, 2007) and play a vital role in carbon cycling for two reasons: firstly, carbon accumulation from plant materials exceeds decomposition rates (a negative feedback to climate warming); secondly, a large quantity of carbon is emitted as CH_4 in peatland regions due to the anoxic environment (a positive feedback to climate warming). Peat accumulation and decomposition rates are influenced by vegetation primary production, soil hydrological conditions, water table position (WTP) and temperature. Among them, WTP, as it determines the transition between aerobic and anaerobic decomposition, is seen as the most important factor (Roulet *et al.*, 2007).

In northern latitudes, peatland formation and development are closely associated with soil freezing-thawing processes. Permafrost formation and degradation change the landscape surface, as well as the peatland hydrology and thermal properties (Wania, 2007). Based on surface hydrology and plant communities, northern peatlands can be divided into two major categories: dry permafrost-plateau palsa and wet fen permafrost-free peatland (Bäckstrand *et al.*, 2010). With permafrost thaw, another type of intermediate bog-like peatland forms, with relatively wetter conditions than the palsa type (Christensen *et al.*, 2012). Generally, drier palsas release the smallest amount of CH_4, while wet fen areas have the highest CH_4 release (Limpens *et al.*, 2008). With continuous permafrost thawing (ground subsidence) and higher runoff in northern latitudes, areal cover of wet fen peatlands is likely to increase (Malmer *et al.*, 2005) which might result in higher CH_4 emissions on short time scales. However, the wetting of peatland may be counteracted by a potential increase in evapotranspiration and the deepening of permafrost with increased vertical drainage in the future (Avis *et al.*, 2011). Another important factor regulating the contribution of peatland-processes to global climate is the areal extent of peatlands. In a recent review, Yu (2012) concluded that carbon fluxes from northern peatlands were largely determined by peatland expansion dynamics (determined using basal ^{14}C dates) during the Holocene. There is still considerable uncertainty regarding the spatial extent of peatlands in the future (Koven *et al.*, 2011).

1.3. Water interactions with the carbon cycle

Generally, terrestrial vegetation growth and carbon cycling are intrinsically coupled with water cycling (Fig. 2). Soil moisture is one of the key factors influencing vegetation growth, plant phenology, nutrient transport and soil respiration. In turn, vegetation influences water cycling through intercepting precipitation (rainfall and/or snow), taking up water through roots, holding more water in soils, and transpiring to the atmosphere. Moreover, vegetation litter layers can increase surface roughness and impact water partitioning between infiltration and surface runoff (Chen *et al.*, 2014).
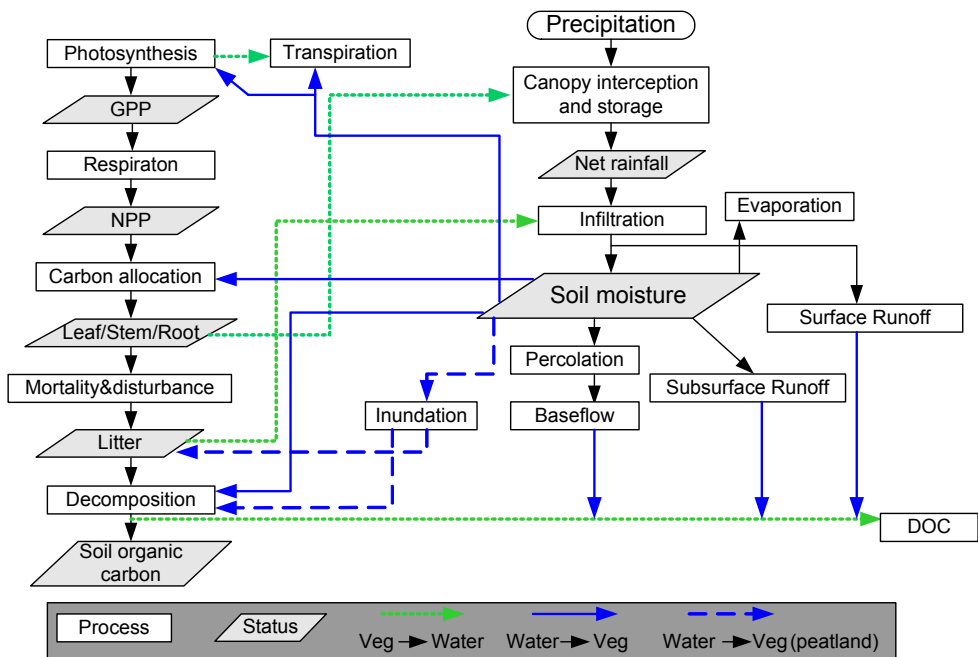
Figure 2. Coupled processes between vegetation (Veg) dynamics/carbon cycling and water cycling (modified from Chen *et al.* (2014)). Blue lines represent hydrological cycles impacting vegetation dynamics and soil carbon cycling; whereas green lines represent vegetation impacts on hydrological cycles.

In northern peatlands, an important characteristic in terms of water interacting with carbon cycling is the soil water inundation mechanism (dashed line in Fig. 2) which determines vegetation composition and strongly impacts the emission of CH_4 as well as ecosystem production and respiration (Watts *et al.*, 2014). Beyond that, a field experiment in Greenland revealed that soil moisture as a driving variable can determine the sink/source sign of the net ecosystem exchange (NEE)

in high-level warming experiments (Sharp *et al.*, 2013) through impacting microbial activities and nutrient cycling. Furthermore, Yi *et al.* (2014) highlighted the importance of spring hydrology in promoting summer net carbon uptake in northern ecosystems. In addition, soil water can greatly influence thermal properties of unfrozen soil, which plays an important role in regulating climate warming effects on permafrost conditions (Wania *et al.*, 2009a).

1.3.1. Terrestrial and aquatic system interactions

Water flow *on* and *through* the terrestrial landscape carrying dissolved organic carbon (DOC) affects water quality, the productivity of aquatic vegetation and microbial activity in aquatic systems (Wrona *et al.*, 2006). Laterally transported DOC from terrestrial to aquatic ecosystems can represent a significant fraction of ecosystem fixed carbon and have significant impacts on aquatic carbon cycling (Freeman *et al.*, 2004). Across large areas of northern latitudes, the DOC concentration has recently increased in streams and lakes (Monteith *et al.*, 2007). With permafrost thaw and runoff responses to climate change, there is a high possibility that previously frozen soils could become hydrologically accessible and water flowing through unfrozen soils may bring out more DOC (Frey & Smith, 2005, Jantze *et al.*, 2013) to downstream aquatic systems. The important roles of inland water in regulating global C cycling was highlighted by Tranvik *et al.* (2009) and the authors pointed out that the carbon emissions from inland waters to the atmosphere are of a similar magnitude to global terrestrial net ecosystem production. Considering the predominant carbon sources originating from terrestrial ecosystems and intense organic carbon mineralization in aquatic systems, it is fundamentally important to accurately quantify the lateral transports of DOC from terrestrial ecosystems.

The riparian zone, as the interface between land and rivers or streams, regulates stream chemistry dynamics (Bishop *et al.*, 2004, Seibert *et al.*, 2009) and also exerts a major control on runoff generation. The riparian zone often has distinct soil (more organic matter near the soil surface) and vegetation characteristics compared to the surrounding landscape. During the high flow season, the generated runoff from upland areas passing through the shallow organic-rich layer in the riparian zone can significantly alter the soil water chemistry compared with the low flow season (Grabs *et al.*, 2012). Due to its hydrological and biogeochemical regulatory function, the riparian zone is recognized as an important area for considering terrestrial and aquatic ecosystem interactions.

1.4. Dynamic ecosystem modelling

Dynamic global vegetation models (DGVMs) are frequently used to investigate the influences of vegetation dynamics and global biogeochemical fluxes on climate change and vice versa. The developments of DGVMs are mainly based on the equilibrium biome models (Prentice *et al.*, 1992), vegetation physiological models (Farquhar *et al.*, 1980, Haxeltine & Prentice, 1996) and biogeochemistry models (Melillo *et al.*, 1993, Parton *et al.*, 1994), but DGVMs were further developed to represent vegetation dynamics as well as dynamic transitions between biomes (Prentice *et al.*, 1993, Smith *et al.*, 2001, Sitch *et al.*, 2003). The Lund-Potsdam-Jena General Ecosystem Simulator (LPJ-GUESS) (Smith *et al.*, 2001) is a DGVM that includes individual-level representations of vegetation dynamics and competition for resources, but which shares some process descriptions with the area-based LPJ-DGVM.

One goal of dynamic ecosystem modelling is to explicitly simulate carbon and water fluxes between atmosphere, vegetation and soils at regional and global scales. The LPJ family of models has often been applied to simulate regional and global carbon fluxes (Ahlström *et al.*, 2012, McGuire *et al.*, 2012), vegetation dynamics (Hickler *et al.*, 2004, Hickler *et al.*, 2012, Miller & Smith, 2012), and water fluxes (Gerten *et al.*, 2004). However, one of the limitations for the regional and/or global carbon budget estimations is that the spatial resolutions are generally too coarse to specifically account for inland water, which often covers quite small extents (Battin *et al.*, 2009). This could result in large uncertainties in regional and global carbon budget estimations, due to the high emissions from inland water that cannot be replaced by terrestrial ecosystem process descriptions. In addition, the independent grid cell simulations in most DGVMs ignore lateral water and mass transports across landscapes (Naden *et al.*, 2000).

1.5. Distributed hydrological modelling and ecohydrological modelling

1.5.1. Distributed hydrological models and topography

To consider water and/or mass flow across landscapes as well as the interactions with aquatic systems, spatially distributed hydrological processes are required to model runoff generation as well as flow routings within certain boundaries (e.g. a catchment). The method of describing distributed hydrological processes varies in the approximation of the flow network and the determining factors for water flow

traveling time, e.g. soil texture, topography, soil freezing and hydrogeology (Döll & Fiedler, 2008). Generally, for global hydrological models, flow routing is linked to a coarse-resolution flow network (Gong *et al.*, 2009), ranging from a few kilometres to a few degrees in spatial extent. The estimated water travelling time can be spatially variable or temporal variable, or both, or be based on global fixed values (Arora & Boer, 1999, Döll *et al.*, 2003, Rost *et al.*, 2008). For catchment hydrology, more spatially explicit hydrological processes have been presented by integrating vegetation influences, soil properties, detailed water paths as well as local climate conditions (Tague & Band, 2004).

Topography describes the shape of the earth surface and plays a vital role in determining surface water movement and in characterising microclimate, affecting vegetation distributions as well as soil moisture conditions (Zinko *et al.*, 2005, Wilson *et al.*, 2007). Topography is often described as the first-order control of lateral water movements and accumulation (Moore *et al.*, 1991, Wilson *et al.*, 2000) and topographical indices are widely implemented at different scales in hydrological models to describe water flow (Beven & Kirkby, 1979, Wigmosta *et al.*, 1994). Based on the implementation schemes of topographical indices in distributing flow, process-based catchment hydrological modelling can generally be divided into two categories: implicit statistical models (Beven & Kirkby, 1979, Tague & Band, 2001) and explicit process-based models (Wigmosta *et al.*, 1994, Tague & Band, 2004). The implicit statistical models often describe lateral water flow by using statistical distributions of saturation deficits across the entire catchment, while the explicit models transfer water explicitly from cell to cell (Tague & Band, 2001). Due to their lower computational requirements, implicit water distribution methods are widely implemented in multiple fields, ranging from modelling soil moisture distribution to ecological applications (Moore *et al.*, 1991, Zinko *et al.*, 2005, Kopecký & Čížková, 2010, Wolf, 2011, Persson *et al.*, 2012). Explicit water distribution methods are generally implemented in regions with sufficient spatial information describing local soil conditions.

1.5.2. Ecohydrological modelling

Most hydrological models have a simplified representation of vegetation or depend on inputs from other models to treat vegetation effects. The emergence of ecohydrological models has overcome this limitation by considering the hydrological interactions with ecological and biogeochemical processes in a hydrological independent unit (Krysanova & Arnold, 2008, Asbjornsen *et al.*, 2011). Current ecohydrological models differ, however, in how they represent the interactions between ecological and hydrological processes. In a recent review by Chen *et al.* (2014), the authors grouped all ecohydrological models into two types:

one-way coupling models and mutual-way coupling models. One-way coupling models, like DHSVM (Wigmosta *et al.*, 1994) and SHE (Abbott *et al.*, 1986), only consider vegetation effects on hydrological cycles (Fig. 2 dashed green lines) without hydrological feedbacks on vegetation dynamics. Mutual-way coupling treats both vegetation influences on hydrological processes and hydrological impacts on vegetation dynamics, e.g., SWAT (Arnold & Fohrer, 2005) and RHESSys (Tague & Band, 2004). However, the mutual-coupling models differ in the complexity of their vegetation dynamics representations. With more complex interactions between hydrological cycling and vegetation dynamics, the models tend to need more computational resources and are therefore more suitable for applications in smaller catchments.

1.6. Linking distributed hydrological processes to dynamic vegetation modelling

Similar to the mutual-way coupling in ecohydrological modelling described above, spatially linking independent units in dynamic vegetation models with hydrological processes enables us to include plant-water interactions. The link also provides a platform to explore ecohydrological feedbacks on other ecosystem processes, e.g. soil biogeochemical processes (D'Odorico *et al.*, 2010). Integrating distributed hydrological processes into a DGVM could provide a complete and consistent estimation of hydrological and carbon cycles, which is of great importance for hydrological and climatically sensitive regions. Furthermore, the carbon cycling in dynamic ecosystem models can, when distributed hydrological processes are included, make it possible to model soil water DOC concentration and catchment DOC exports. Until now, only very few ecosystem models have attempted to integrate DOC dynamics with terrestrial C cycling (Parton *et al.*, 1994, Currie & Aber, 1997, Neff & Asner, 2001, Michalzik *et al.*, 2003, Wu *et al.*, 2013), and the processes in these models vary widely in degrees of complexity, especially for soil-specialized DOC models. Most importantly, the dynamics of vegetation (e.g. resource competition, mortality, and disturbance) are generally not explicitly represented.

2. Aims and objectives

The aim of this PhD thesis is to quantify and evaluate the impacts of hydrological processes on ecosystem vegetation dynamics and carbon cycling at a catchment scale. The considered hydrological processes include spatial water movements *on* and *through* the landscape and hydrological mass (DOC) transport within the catchment boundary. By integrating these spatially distributed hydrological processes into the dynamic ecosystem model LPJ-GUESS, we can integrate both vertical (atmosphere-vegetation-soil) and horizontal carbon fluxes (DOC export) and then assess the catchment carbon budget. To achieve this aim, the study is divided into the following four steps:

1. To extend one-dimensional water flow modelling among atmosphere-vegetation-soil in LPJ-GUESS to three-dimensional water flow through the landscape within the catchment boundary based on topographical indices, and to further evaluate the impacts of the integrated distributed hydrological processes on ecosystem-level carbon fluxes (Papers I & II);

2. To investigate the potential influences of integrating different flow algorithms on modelled hydrological and carbon fluxes in the catchment (Paper II);

3. To build up a catchment-level carbon budget by integrating both terrestrial and aquatic system carbon fluxes and to investigate the interacting dynamics of different carbon components and their contributions to the catchment carbon budget in a warming future (Paper III);

4. To dynamically model soil water DOC concentration as well as DOC routing within the catchment and to link soil DOC exports with vegetation composition, soil organic carbon (SOC), soil properties and hydrological conditions (Paper IV).

3. Study area and data

3.1. Stordalen catchment

The Stordalen catchment (covering 16 km^2) is located in northern Sweden (Fig. 3) and situated 9.5 km east of the Abisko Naturvetenskapliga Station (ANS, Abisko research station). The catchment is in the discontinuous permafrost zone and permafrost is mainly found in the palsa peatland located at lower elevations. The topography of the catchment is dominated by a north-facing mountainside in its southern part, with lower flat region in the northern part. The mean air temperature was –0.7^{o}C for the period 1913-2002 (Christensen *et al.*, 2004) and 0.49^{o}C for the period 2002-2011 (Callaghan *et al.*, 2013) based on the ANS records. Mean annual precipitation increased from 304 mm for 1961-1990 to 362 mm for 1997-2007 (Margareta *et al.*, 2013), followed by very low precipitation (254 mm on average) for 2008-2010 (Paper IV). The land cover types consist of tundra heath, birch forest, dry palsa, semi-wet bog-like *Sphagnum* peatland, wet fen *Eriophorum* peatland, rivers and lakes. The detailed species found in this catchment are listed in Paper III.

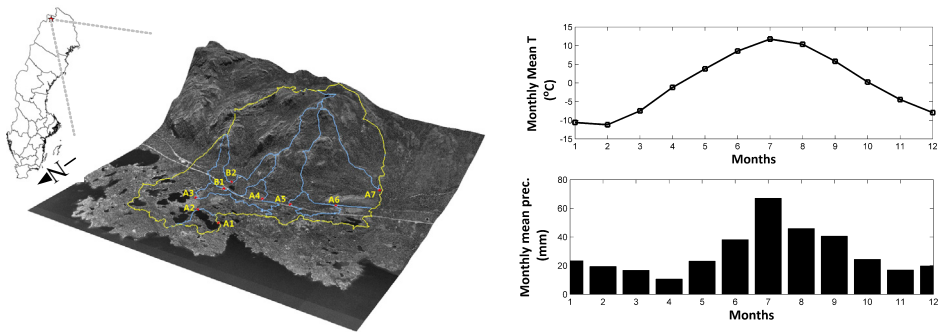**Figure 3**. Location of the Stordalen catchment and a digital elevation model (DEM) map with a draped aerial photograph are shown on the left (elevation is enhanced three times for visual effect). The monthly average temperature (T) and precipitation (prec.) for the period of 2001-2012 are shown on the right panel (Paper IV). Each dot in the map represents a DOC and runoff observation point (Paper I, II and IV).

3.2. Climate data and other inputs

To run LPJ-GUESS for the Stordalen catchment, a high spatial resolution (50 m) climate dataset were used in Papers I-IV. The monthly temperature at 50 m resolution for 1913-2000 were developed by Yang *et al.* (2011) and the development of these data was based on a wide range of observations from the weather stations near ANS, local temperature measurements as well as considering the effects of the Torneträsk lake close to the catchment. The monthly precipitation and cloudiness data (1913-2000) at 50 m resolution were downscaled (bilinear interpolation) from 10 min resolution using CRU TS 1.2 data (Mitchell *et al.*, 2004). During the downscaling process the precipitation data were corrected by considering the influences of topography as well as using historical measurements of precipitation from the ANS records. In Paper I, the simulated historical period is from 1913 to 2010 and additional ten years (2001-2010) of precipitation data were obtained from ANS. The precipitation data were interpolated to the whole catchment according to the observation that annual precipitation increases by 6.5% for every 100 m of altitude (Olefeldt *et al.*, 2013). The monthly temperatures for 2001-2010 in Paper I were determined by applying temperature anomalies from the output of the Rossby Centre Atmosphere Ocean (RCAO) regional climate model for a grid cell near Stordalen to the 50 m resolution climate data. In Paper II-IV, two more years (2011-2012) of monthly precipitation data as well as twelve years (2001-2012) of monthly temperature data were further collected and used. In Papers I-IV, the monthly cloudiness data for 2001-2012 were simply repeated using the forcing from 1990 to 2000. Additionally, annual atmospheric CO_2 concentrations for the period 1913-2010 were also used and based on (McGuire *et al.*, 2001) and TRENDS (http://cdiac.esd.ornl.gov/trends/co2/contents.htm). In Paper III, a future scenario was applied and was based on the anomalies (including temperature, precipitation and cloudiness) between the simulated outputs from RCAO and the historical dataset at 50 m resolution. The RCAO climate data was downscaled for the Arctic region using boundary forcing from a general circulation model forced by the A1B SRES emission scenario for 2013-2080 (Zhang *et al.*, 2013). A DEM was provided by the National Land Survey of Sweden and was used in Papers I-IV to calculate topographic indices. A soil map in vector format was provided by the Geological Survey of Sweden and was used to identify different soil types in Papers I-IV.

3.3. Calibration and evaluation data

In this thesis, a wide range of observation data from the Stordalen catchment were used (Table 1) to calibrate and evaluate the model's performance. The majority of data were collected during 2001-2012.

Table 1. Summary of the observation data used in Papers I-IV to evaluate model's performance. The climate forcing data are not presented here.

Data	Time period	Location	Reference	Paper
Daily runoff at sampling points	2007-2009	Distributed points	(Olefeldt *et al.*, 2013)	**I&II**
Digitized vegetation map	1997	Whole catchment	National Land Survey of Sweden	**I**
Daily water table position (WTP)	Summer season 2003-2012	Stordalen peatland	(Petrescu *et al.*, 2008)	**II**
Eddy Covariance-NEE	2006-2008	Wet fen *Eriophorum* peatland	(Christensen *et al.*, 2012)	**II&III**
Dark Chamber respiration	Summer season 2004-2005 and 2007-2008	Stordalen peatland	(Bäckstrand *et al.*, 2010)	**II**
Active layer depth	September 1978-2011	Storflaket peatland	(Åkerman & Johansson, 2008)	**II**
Eddy Covariance-NEE	2008-2009	Palsa/*Sphagnum* peatland	(Olefeldt *et al.*, 2012)	**III**
Eddy Covariance-CH$_4$	2006-2007	Wet fen *Eriophorum* peatland	(Jackowicz-Korczyński *et al.*, 2010)	**III**
Eddy Covariance-NEE	2007-2010	Birch forest	(Heliasz, 2012)	**III**
Analysed DOC concentration	2008	Stordalen peatland	(Olefeldt & Roulet, 2012)	**III**
Analysed DOC concentration and export	2007-2009	Distributed points	(Olefeldt *et al.*, 2013)	**III&IV**
Analysed DIC export	2007-2009	Distributed points	(Olefeldt *et al.*, 2013)	**III**
Catchment-level CO$_2$ and CH$_4$ emissions from lakes and rivers	2008-2011	Whole catchment	(Lundin *et al.*, 2013)	**III**

4. Methods

4.1. LPJ-GUESS and LPJ-GUESS WHyMe

LPJ-GUESS is a climate-driven and process-based dynamic ecosystem model which includes explicit representations of vegetation dynamics (derived from a forest gap model, Smith *et al.* (2001)) and soil biogeochemistry (Sitch *et al.*, 2003). The forest structure and dynamics in LPJ-GUESS are represented by plant functional types (PFTs) of different age classes (cohorts) competing for light and soil resources within different replicate patches in each grid cell (Smith *et al.*, 2014). PFTs are used to group plants on the basis of their physiological, phenological and morphological characteristics (Wolf *et al.*, 2008b, Hickler *et al.*, 2012). Three soil carbon pools are distinguished based on their different prescribed turnover rates: litter, fast and slow soil organic matter pools (Sitch *et al.*, 2003). The model distinguishes processes occurring at different time-scales. For instance, photosynthesis, respiration and soil decomposition are modelled on daily basis/step, whereas plant growth, vegetation dynamics (mortality, establishment and disturbance) and carbon allocation are modelled on annual basis/step (Hickler *et al.*, 2004). Recently, nitrogen (N) cycling and N limitation on plant production have also been included in a version of LPJ-GUESS (Smith *et al.*, 2014).

Water cycling between atmosphere-vegetation-soil is described in Gerten *et al.* (2004) and the modelled water processes include vegetation interception, transpiration, infiltration, percolation, soil evaporation and runoff (Fig. 4, vegetation water balance). Vegetation-intercepted water amount is a function of plant functional types (PFTs), leaf area index (LAI) and precipitation, whereas vegetation transpiration water is the smaller value of atmospheric-demand and plant-controlled-supply. The plant-controlled-supply is related to PFTs root distribution and soil water content (Sitch *et al.*, 2003). Soil evaporation occurs on bare ground and is a function of soil water content. Before estimating soil evaporation, if the infiltrated/percolated water amount plus the antecedent soil water is in excess of soil water holding capacity, surface and subsurface runoff will be generated.
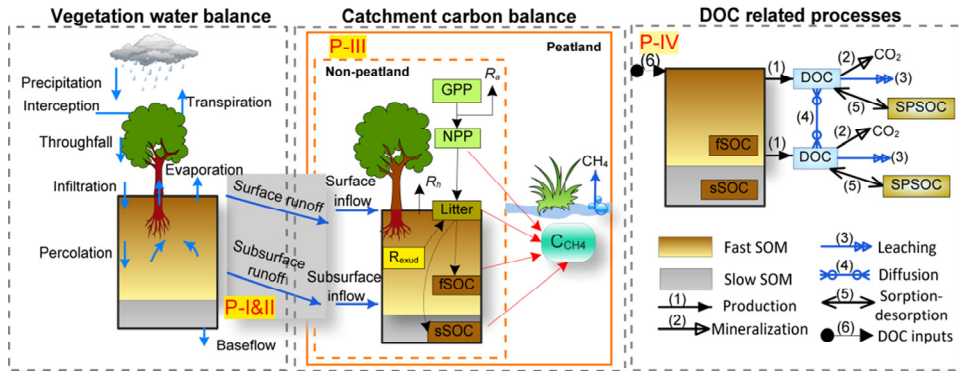
Figure 4. Schematic diagram of water and carbon cycling in LPJ-GUESS and/or in LPJ-GUESS WHyMe. The model developments included in this thesis are also presented. The four papers in this thesis are denoted with P-I, P-II, P-III, P-IV.

An Arctic-enabled version of LPJ-GUESS (henceforth referred to as LPJ-GUESS WHyMe) has been developed (Miller & Smith, 2012) by including the soil permafrost, peatland vegetation and peatland hydrology descriptions first included in LPJ-WHyMe (i.e. LPJ-DGVM with Wetland Hydrology and Methane) (Wania *et al.*, 2009a, 2009b, 2010) (Fig. 5). The mineral soil hydrology mainly follows the standard LPJ-GUESS scheme described above. However, the peatland hydrology has been adapted to use an acrotelm-catotelm soil structure (Granberg *et al.*, 1999), assuming a permanently inundated body of peat underlying the top 0.3 m, down to 2 m depth (extended from 1.5 m soil depth in LPJ-GUESS), while the top 0.3 m has a fluctuating water table. In addition, standing water (up to 100 mm) is allowed for peat soils. In LPJ-GUESS WHyMe, the soil temperature at each 100 mm soil layer is updated daily using the Crank-Nicolson algorithm (Crank & Nicolson, 1996) for both mineral and peatland soils, and takes into account the effect of soil water freezing and thawing. This adds soil freezing effects to water and carbon cycling. In addition, two new peatland PFTs and a vegetation inundation stress mechanism have been updated in LPJ-GUESS WHyMe. To account for the methane (CH_4) that is mainly released from peatland, an extra carbon pool for methanogens has been added in LPJ-GUESS WHyMe (Wania *et al.*, 2010). The main source for this carbon pool includes root exudates and easily-decomposed materials (Fig. 4, peatland in the catchment carbon balance box).

Both LPJ-GUESS and LPJ-GUESS WHyMe remove the generated runoff from the model domain without considering interactions with downslope grid cells, which is crucial for consideration of spatial variability of soil moisture and hydrological and carbon fluxes at the catchment scale (Tague & Band, 2001, Wolf, 2011). Therefore, a main focus of this thesis has been to describe lateral water

16

movement between grid cells within the catchment boundary (see P-I&II in grey-shaded area, Fig. 4).
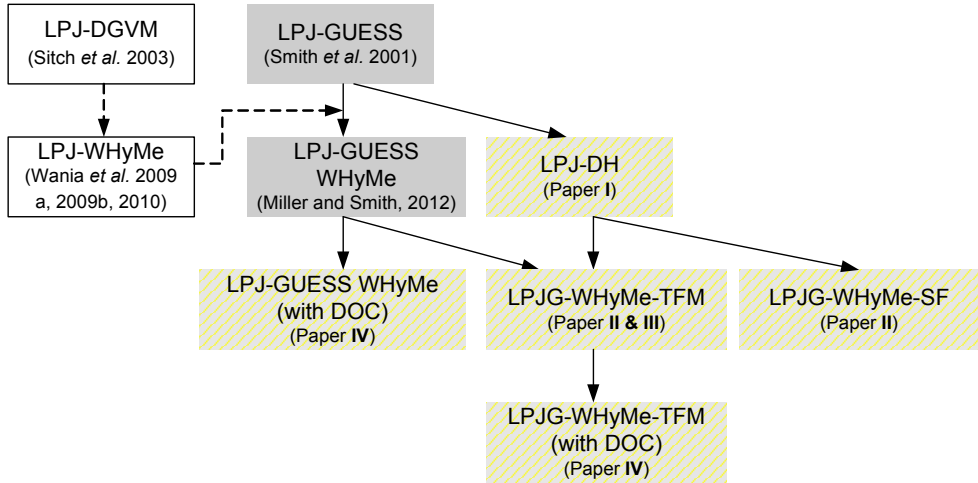

Figure 5. Flowchart of the related model developments and the corresponding model names. The model descriptions can be found in each specified reference.

4.2. Topographical-indices based hydrological scheme

A distributed hydrological scheme has been proposed and implemented within the framework of LPJ-GUESS (Paper I). The scheme utilizes three topographical indices to partition flow and determine flow routing in the catchment. The three indices used in the model are drainage area (*DA*), flow direction (*Fdir*) and slope (*S*) (Fig. 6a). The indices were extracted from the DEM at 50 m resolution and a single flow (SF) algorithm was chosen to estimate the indices (O'Callaghan & Mark, 1984). The values of *DA* determine how many upslope cells drain to a specific cell as well as the runoff accumulation order for each day (colour bar in Fig. 6b). Moreover, *Fdir* connects each grid cell with its neighbouring cells by lateral surface flow (arrows in Fig. 6b) and the value of *S* influences runoff generation. This steady-state information about flow sequences (*DA*), cell connections (*Fdir*) and slope (*S*) are used as grid cell input attributes to LPJ-GUESS (Fig. 6a). To achieve flow accumulation within the catchment boundary at a daily time scale, the simulation order in LPJ-GUESS was changed from cell-by-cell to day-by-day. At the end of each day, the generated surface runoff flows to the pointed neighbouring downslope cell. For the whole catchment, water

accumulation starts from the catchment divide and ends at the catchment outlet (Fig. 6b).
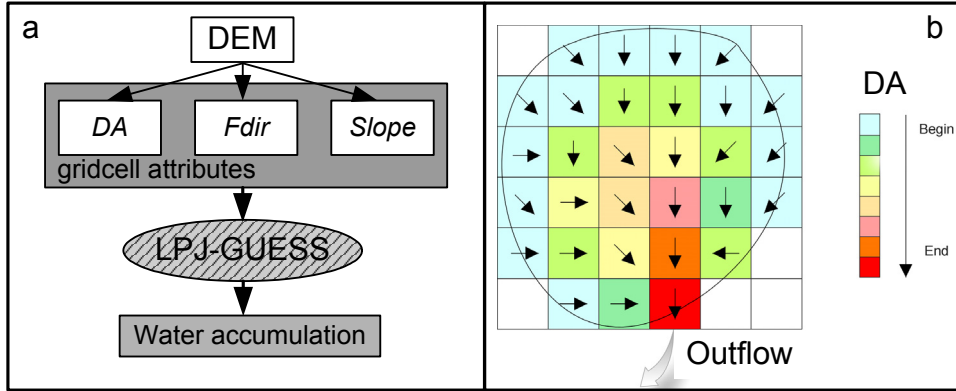

Figure 6. Flowchart of integration of topographical indices into LPJ-GUESS (a) and schematic illustration of cell-to-cell flow accumulation within the catchment boundary (b) (modified from Fig. 1 in Paper I).

4.3. Flow algorithms comparison

The flow algorithm chosen to estimate topographical indices in Paper I is D8, (O'Callaghan & Mark, 1984) which is one of the most widely-used SF algorithms (Fairfield & Leymarie, 1991, Costa-Cabral & Burges, 1994, Orlandini *et al.*, 2003). Generally, SF algorithms only consider parallel flow and flow convergence, which may not produce realistic flow patterns. Another group of flow algorithms are the multiple flow (MF) algorithms, where both flow divergence and convergence are considered (Seibert & McGlynn, 2007, Zhou *et al.*, 2011, Pilesjö & Hasan, 2014). Existing MF algorithms differ mainly in how they partition the flow to multiple downslope cells, which could cause the estimation of flow pathways to vary to a large degree. A recently-developed Triangular Form-based Multiple (TFM) flow algorithm (Pilesjö & Hasan, 2014) agrees more closely with theoretical estimations of specific catchment area (SCA) compared with other MF algorithms. By dividing a grid cell into eight planar triangular facets, the TFM algorithm can deal with the detailed topographical variations within grid cells. Water flow from each facet can be routed to other facets in the same grid cell or to neighbouring cells (Pilesjö & Hasan, 2014). Furthermore, the flow estimation over flat surfaces has also been improved (Hasan *et al.*, 2012). Therefore, one SF (D8) and one MF (TFM) algorithm were incorporated into LPJ-GUESS WHyMe to compare and

evaluate the influence of different flow distribution on modelled catchment hydrological and carbon fluxes.

In contrast to the SF algorithm implementation on the LPJ-GUESS platform, the TFM algorithm-extracted *Fdir* of a specific cell may connect to multiple neighbouring cells. Therefore, flow partition fractions to multiple neighbouring cells are recorded for each grid cell. All the model settings and input data are kept the same except for the use of different flow algorithms to derive topographical indices to describe flow in the model (Paper II). Additionally, the subsurface lateral flow is modelled based on the quasi three-dimensional saturated ground flow algorithms (Wigmosta *et al.*, 1994). The grid cell flow connectivity is kept the same as surface flow for both the SF and the TFM algorithms, assuming the slope of the hydraulic head is parallel to the ground surface. A variety of observed data, including runoff, WTP, peatland net ecosystem exchange (NEE) and soil respiration, have been used to evaluate the differences generated from the two flow algorithms.

4.4. Catchment carbon budget

The catchment is a hydrological unit and is separated from neighbouring areas by its watershed boundary. It is commonly assumed that there is no lateral water flow from outside the boundary into the catchment. Each drop of precipitation that is not stored, evaporated or transpired, will travel within the catchment and reach the catchment outlets. From a carbon budget perspective, the estimation of a carbon budget using the catchment as a unit (Paper III) can assume that there are no lateral waterborne carbon fluxes into the catchment and the catchment unit can be viewed as a closed system where no lateral water flow from outside the catchment can influence vegetation and the carbon cycle. Furthermore, with the availability of observed CO_2 and CH_4 fluxes from lakes and rivers (Lundin *et al.*, 2013) in the Stordalen catchment, the carbon fluxes from the aquatic systems can also be included and scaled to the catchment-level carbon budget. The model simulates catchment vegetation composition as well as dynamics and the annual carbon fluxes from different vegetation classes are proportionally integrated into the catchment carbon budget based on the modelled vegetation distribution.

4.5.   Simulations with high spatial resolution

Subarctic ecosystems are characterized by small-scale variations in vegetation composition, hydrological conditions, nutrient status and carbon fluxes (Lukeno & Billings, 1985, McGuire *et al.*, 2002, Callaghan *et al.*, 2013). Therefore, modelling exercises aiming to investigate carbon cycling in this type of complex ecosystem strongly require process simulations and climate driven data at high a spatial resolution. In contrast to conventional approaches using outputs from the Regional Climate Model (RCM) or Global Circulation Model (GCM) as climate inputs to run LPJ-GUESS (Koca *et al.*, 2006, Morales *et al.*, 2007, Ahlström *et al.*, 2012), the model applications involved in this thesis are driven by 50 m resolution climate data (Yang *et al.*, 2011) and the spatial resolution of the DEM is consistent with the climate data (see Section 3.2). The 50 m air temperature data have integrated the effects of large lakes (Torneträsk for Stordalen catchment), solar radiation, and sub-grid topographical variations on air temperature patterns. Without these high spatial resolution climate data, it would be impossible to implement our distributed hydrological scheme at the catchment scale (Paper I-IV) and especially to capture the small-scale peatland vegetation dynamics (Paper III).

4.6.   Soil organic carbon profiles and riparian zone

Soil organic carbon (SOC) profiles in boreal and polar soils are generally characterized by higher SOC content concentration towards the surface compared with a more evenly distributed SOC profile in tropical and temperate soils (Lawrence & Slater, 2008). Soil organic carbon (SOC) provides the primary source for DOC production (Hagedorn *et al.*, 2004) and DOC exports are influenced by microbial activity, soil texture, hydrological conditions and temperature. These drivers may vary with soil depth, so modelling DOC fluxes requires a finer, vertically-resolved SOC profile.

In LPJ-GUESS, fast and slow soil carbon pools are evenly distributed in mineral soils. In paper IV, a modification of SOC vertical profiles for mineral soils has been implemented based on a log-log function from Jobbágy and Jackson (2000). The SOC fraction (%) in each 100 mm soil layer is estimated and implemented in the model (Paper IV). Different decrease rates of SOC fractions from soil surfaces have been assigned to tundra heath, birch forest and riparian soil types (Fig. 7a). For mineral soil, the amount of fast SOC (fSOC) is firstly distributed in top soil layers until its maximum depth. Thereafter, slow SOC (sSOC) is distributed in each soil layer down to the bottom layer (Fig. 4, DOC related processes box). For

peatland, fast and slow soil carbon pools are explicitly assigned to the actotelm and catotelm layers, respectively.

To reflect the influence of the riparian zone on catchment-level DOC exports (Paper IV), the identification of the riparian zone in the catchment is based on empirically setting a threshold value (DA = 120) for the estimated DA based on the TFM algorithm. All grid cells with DA values higher than this threshold value and not considered as peatland soil types, are grouped as riparian grid cells. The SOC profile distributes a higher fraction of SOC in the top layers for riparian zone soils (Figure 7a) and assumes more organic material soils.
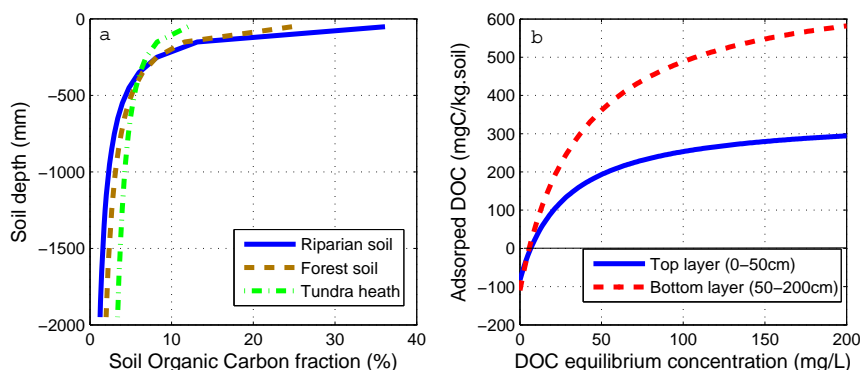

Figure 7. Mineral soil organic carbon profiles (a) and a modified Langmuir sorption isotherm (b) based on Paper IV.

4.7. Soil water DOC and lateral transport

The modelling of DOC dynamics in LPJ-GUESS WHyMe includes five key processes (Fig. 4, DOC related processes box): DOC production, mineralization, sorption-desorption, diffusion and export (Paper IV). Two new soil carbon pools were added for the two soil layers: a DOC pool where organic carbon is dissolved in soil water, and a sorbed potentially soluble organic carbon (SPSOC) pool. Daily DOC production and mineralization rates are calculated based on the carbon pool size (fSOC and sSOC pool sizes for DOC production and DOC and SPSOC pool size for mineralization), a Q_{10}-based relationship for soil temperature responses and the basal microbial production or mineralization rate at 20$^{\text{o}}$C (Yurova *et al.*, 2008). The diffusion processes between the upper layer (acrotelm layer for peatland) and lower layer (catotelm layer for peatland) is driven by soil water DOC concentration gradients. Furthermore, a modified Langmuir sorption isotherm is implemented for mineral soils (Lilienfein *et al.*, 2004) to describe the

21

sorption and desorption processes between the DOC and SPSOC carbon pools (Fig. 7b). For peatland, the sorption and desorption between DOC and SPSOC carbon pools were implemented as a linear equilibrium process. The modelled DOC export from the soil column is a function of daily runoff and soil DOC concentration. The lateral transport of DOC is determined by flow accumulation and distribution on a daily basis and the amount of water that can accumulate determines the amount of DOC that can be retained in each grid cell.

4.8. Parameterization and sensitivity testing

The parameterisation of saturated hydraulic conductivity (Ks) and the decay rate (f) with soil depth in Paper II was based on a quasi-random parameter sampling from the ranges obtained from the literature (Clapp & Hornberger, 1978, Freeze & Cherry, 1979, Famiglietti *et al.*, 1992). The parameter combination that resulted in the lowest overall relative root mean square error (RRMSE) at the six observation points was selected (Paper II, Appendix). In paper IV, a sensitivity analysis (SA) was conducted for three upland grid cells with different climate conditions and one peatland grid cell in the catchment to test the influence of DOC-related processes (Fig. 4) on soil water DOC concentration. The variance-based Sobol sensitivity index (Saltelli *et al.*, 2008) was chosen to quantify the newly-added parameters' contributions to the DOC concentration (Paper IV, Grid cell-level SA Section). The first-order Sobol index quantified each parameter's contribution to the variance of DOC concentration while the total Sobol index described the overall parameter importance by including each parameter's interactions with other parameters. By estimating Sobol indices for each parameter, the most influencial parameters for DOC exports could be identified. Thereafter, these paramters could be (randomly) sampled further for the catchment-level DOC export. Observed DOC export data were used to evaluate the model estimations.

5. Results and discussion

The main aim of this thesis is to explicitly explore different perspectives regarding hydrological process interactions with vegetation dynamics and carbon cycling in northern latitudes. To achieve this aim, a distributed hydrological approach has been proposed within the framework of the dynamic ecosystem model LPJ-GUESS (WHyMe). This was applied in an accessible subarctic Stordalen catchment in northern Sweden, where intense observations have been undertaken over a long time period. One of the important results arising from this work was that lateral water and DOC transports cannot be ignored when modelling ecosystems' water and carbon dynamics, especially in a climatically sensitive environment. In this thesis, the consequences of integrating lateral and vertical water movements were extensively evaluated using the widely available observation data from the Stordalen catchment. A summary of the results is presented in the following sections.

5.1. From topographical variations to water partitioning and lateral movement (Paper I)

To build up the missing component of considering water interactions between grid cells in LPJ-GUESS, a distributed hydrological scheme for implementing lateral water flow from cell to cell was proposed in Paper I. The developed model was named LPJ-Distributed Hydrology (LPJ-DH). The proposed scheme explicitly considered the topographical effects in determining runoff generation and lateral flow accumulation. The incorporated indices DA and S are the main components for the frequently-used topographical wetness index (TWI, ln(DA/tan(S))) (Beven & Kirkby, 1979). However, the explicit cell-to-cell routing method in our approach avoids the conventional, statistical way of using TWI to implicitly distribute water within the catchment. The extended model LPJ-DH was tested in the Stordalen catchment and comparisons of the modelled and the observed runoff at monthly and annual timescales showed the improved accuracy of runoff estimations as a result of considering topographical variations in the model. The spatial pattern of the runoff also showed the advantage of incorporating

topographical variations in the model; especially increasing the runoff estimations for the steeper areas of the catchment and in the low-lying peatland region. In Paper I, the focus was on the differences between LPJ-GUESS and LPJ-DH and no field measured biomass and carbon fluxes were used. The improved hydrological process descriptions in the catchment resulted in a significant increase in birch forest biomass and in a decrease in tundra summer-green shrub (< 2 m) biomass when comparing the average estimations over the simulation period (1913-2010) from LPJ-DH and LPJ-GUESS. The modelled soil carbon fluxes also showed a statistically significant response to the lateral flow in the catchment, which is in agreement with previous studies (Yurova *et al.*, 2007, Wolf, 2011).

The method proposed in Paper I is straightforward to implement and showed both the benefits of modelling hydrological fluxes and the statistically significant impacts on modelled ecological processes in the model. This implementation can be easily transferred to other ecosystem models where only vertical water movement has been considered. This is of importance in both hydrological and ecological perspectives (Naden *et al.*, 2000). Another potential benefit of the cell-to-cell routing method in Paper I is the effectiveness of capturing variable contributing areas, which is crucial when implementing flow routing for dry seasons or arid/semi-arid regions where limited water flow is only routed locally (Tague & Band, 2001, Sponseller & Fisher, 2008). This is impossible to capture in the statistical-based flow distribution models (Beven & Freer, 2001, Wolf, 2011). However, the proposed distributed hydrological scheme could result in an increase in model simulation time and memory demands, since all grid cells connected to each other are updated at each time step before moving to the next time step. Nonetheless, a semi-parallel simulation strategy in which grid cells with or without inflow run separately could improve the model efficiency.

5.2. From different flow routing to ecosystem carbon fluxes: the importance of considering water flow algorithms (Paper II)

In paper II, the effects of two flow algorithms on catchment hydrological and carbon fluxes were evaluated. Two sets of topographical indices calculated by the SF and TFM algorithms were integrated into LPJ-GUESS WHyMe to describe water routing in the Stordalen catchment. The new models were renamed to LPJG-WHyMe-SF and LPJG-WHyMe-TFM (Fig. 5). The results revealed that the TFM captured water transport amount across the landscape better than the SF algorithm.

The advantages of the TFM algorithm are mainly linked to the flow partitioning to multiple downslope cells as well as the modelled flow over flat regions. The evaluation of the influence of these two flow algorithms on estimating peatland NEE and respiration strongly indicates that the convergent way of driving flow accumulation in the SF algorithm could result in overall overestimations of vegetation uptake and soil respiration.

To our knowledge, this is the first study that evaluates the influence of different flow algorithms, not only on hydrological processes, but also on ecosystem carbon fluxes. It highlighted the importance of choosing appropriate flow routing algorithms, especially within hydrologically and climatically sensitive environments. Furthermore, in Paper II we only focus on evaluating the effects of two flow routing algorithms on the low-lying peatland carbon cycling. However, the impacts of flow routing algorithms on lateral redistribution of dissolved carbon and nutrients should also be considered (Hwang *et al.*, 2012). Although the evaluations of these two flow algorithms may be influenced by the model structure, the results demonstrate the necessity of considering the potential consequences of different flow algorithms.

5.3. From catchment water cycling to catchment carbon cycling: the importance of considering vegetation dynamics and carbon fluxes at a high spatial resolution (Paper III)

In Paper III, a catchment-level carbon budget was built using the extended model LPJG-WHyMe-TFM described in Paper II. The catchment carbon budget integrated the modelled carbon fluxes from different vegetation communities with the observed fluxes from the rivers and lakes. The catchment DOC export was empirically estimated based on the observed DOC concentration with the modelled runoff for birch forest areas.

This is the first process-based model study of the temporal evolution of a catchment-level carbon budget at a high spatial resolution (50 m). The model was shown to be able to capture the seasonality and magnitude of the observed carbon fluxes for different vegetation micro-types (mountain birch forest, tundra heath, *Eriophorum* peatland and *Sphagnum* peatland) within the catchment. The birch forest, the dominant vegetation in the Stordalen catchment, contributed significantly to the inter-annual variation of the catchment carbon budget. However, we note that to accurately estimate the carbon functioning of birch forest

in this region, the model should explicitly consider insect disturbance. The birch forest is cyclically disturbed by autumn larvae and winter moths (Heliasz *et al.*, 2011), which can fundamentally shift the carbon uptake ability of the birch forest. For the catchment peatland, the wet *Eriophorum* peatland showed stronger annual uptake than the relatively drier *Sphagnum* peatland, which is consistent with the observed relative differences between these two types of peatland (Christensen *et al.*, 2012, Olefeldt *et al.*, 2012). For the tundra heath, a relatively smaller uptake was modelled, (however, with a large variability), which is consistent with field observations (Fox *et al.*, 2008).

A future climate scenario with a $2^{o}C$ temperature increase and doubled atmospheric CO_2 concentration since 1960 has been tested for the catchment and the results indicated that the whole catchment will become a much stronger carbon sink by 2080, mainly due to a stronger carbon uptake by, and wider distribution of, birch forest in a near future. To date, however, there is no clear evidence of significant CO_2 fertilization effects in this region (Oechel *et al.*, 1994, Gwynn-Jones *et al.*, 1997, Olsrud *et al.*, 2010), mainly due to the complex interactions between nutrient supplies, UV-B exposure, temperature and growing season length and forest longevity. Therefore, in this paper we further tested the model's sensitivity to the atmospheric CO_2 concentration and found that the CO_2 trajectory dramatically impacts the carbon uptake in the birch forest and tundra heath. This can totally shift the balance of the catchment global warming potential (GWP) resulting from carbon uptake in the birch forest and tundra heath, and the peatland CH_4 emissions.

Consideration of vegetation dynamics and the application of the model at a high spatial resolution showed the detailed vegetation succession (e.g. birch forest encroachment on tundra heath) as well as the carbon flux dependencies on the responses of trees and shrubs to climate drivers at a fine scale. This study also highlighted the urgent need to quantify and understand the CO_2 fertilization effects on the various vegetation micro-types, particularly for tall vegetation types in this region (Olsrud *et al.*, 2010). This application also reveals the complexity of carbon cycling in subarctic ecosystems (Callaghan *et al.*, 2013), and points out some key remaining model developments needed to improve our understanding of complex subarctic ecosystems such as Stordalen's. The necessary developments include nutrient limitation, herbivory and other disturbances, peatland expansion, and aquatic system flux dynamics. With the abundance of observation data in the Stordalen catchment, the improved understanding and the quantified carbon functioning from different vegetation communities can be applied to large areas where large C stocks exist but long term measurements are lacking.

5.4. From water flow to hydrological mass transport: the importance of modelling DOC dynamics (Paper IV)

The estimated dissolved organic carbon (DOC) export in Paper III was based on the modelled runoff and the observed DOC concentration and there is no process-based description in the model. To better quantify DOC losses from terrestrial ecosystems, including its climate and parameter sensitivity, and to understand the dynamic contributions to the whole carbon budget (Paper III), it is necessary to mechanically describe the DOC-relevant processes in soils and to link these processes to the vegetation dynamics and the turnover of the long-term soil carbon pool. In Paper IV, we proposed a set of DOC-related processes in LPJ-GUESS WHyMe and LPJG-WHyMe-TFM (Fig. 5), including DOC production, mineralization, diffusion, sorption-desorption and export/leaching based on previous work by Yurova *et al.* (2008) and Omstedt *et al.* (2012). The proposed processes represent a generalized approach to the dynamic modelling DOC fluxes and have a straightforward link to other ecosystem processes as well as soil properties (Neff & Asner, 2001). Our sensitivity analysis indicated that the DOC production from the SOC and DOC/SPSOC mineralization to CO_2 are the two dominant processes controlling soil water DOC concentration, which is line with several lab experiments (Hagedorn *et al.*, 2004, Kalbitz & Kaiser, 2008). However, there are also different opinions about the dominant processes related to soil DOC concentrations, mainly due to the different time scales considered in various studies. Some processes, like fresh litter decomposition, can happen on the order of hours or faster, which is less than the daily resolution used in our model (Kalbitz *et al.*, 2000, Fröberg *et al.*, 2007).

The catchment-level DOC simulation including DOC routing within the catchment has revealed the high spatial heterogeneity of DOC transport through different land cover types. The estimated DOC export at six points, compared with the observed DOC export data showed the model's ability in capturing DOC flux seasonality. Among the existing land cover types in the catchment, the *Eriophorum* peatland shows the highest DOC export (Olefeldt & Roulet, 2014), followed by the riparian zone and the birch forest. The *Sphagnum* moss areas show the lowest DOC fluxes due to the limited hydrological transport and the lowest litter inputs (Limpens *et al.*, 2008). The important roles of the riparian zone and *Eriophorum* peatland in regulating catchment DOC export are well established (Bishop *et al.*, 2004, Olefeldt & Roulet, 2014). However, at the current model development stage, the riparian zone's specific hydrological processes and vegetation are not yet fully described, which may bring additional uncertainty in terms of the functioning of riparian zone (Laudon *et al.*, 2011).

This is the first model study to integrate dynamically DOC fluxes into a dynamic vegetation model and to consider spatially varying DOC exports from diverse land cover types at the catchment scale. Even though the soil structure and biogeochemical processes are not compatible with other soil-specialized DOC models (Parton *et al.*, 1994, Sollins *et al.*, 1996), the current implementation indicated that DOC-related processes in the framework of LPJ-GUESS WHyMe are at an appropriate level of complexity to represent the main mechanisms of DOC dynamics in soils.

6. Conclusions

In this thesis, a series of model implementations, improvements and experiments have been conducted, including the development of topography-based water flow routing within a dynamic ecosystem model, the evaluation of the influences of lateral flow on eco-hydrological processes and the formulation of a framework explicitly considering DOC dynamics within the catchment. These implementations give us new and important insights into the links between topography-controlled spatial hydrological conditions and ecosystem biogeochemical dynamics.

The following conclusions can be drawn from this thesis:

- Topographical indices can be straightforwardly implemented into dynamic ecosystem models to effectively capture both spatial and temporal variations in hydrological processes.

- The choice of different flow routing algorithms to describe catchment flow patterns does matter for the modelled accuracy of hydrological fluxes, but also for vegetation and carbon dynamics.

- Hydrological conditions are one of the key factors influencing peatland carbon fluxes, especially in determining the amount of carbon released as CH_4. There is therefore an urgent need to accurately represent both vertical and horizontal water fluxes in peatlands.

- According to our model simulations, the role of the subarctic regions as a future sink or source of carbon is largely regulated by the long-term CO_2 fertilization effects on tall vegetation, like shrubs and birch forest. Thus, long-term observations and/or Free Air CO_2 Enrichment (FACE) manipulations are needed in these regions.

- The *Eriophorum* peatland was identified as the hotspot of DOC export in the Stordalen catchment. In a warming future with a large degradation of permafrost in this region, the DOC fluxes, particularly from the *Eriophorum* peatland, could be dramatically increased if the peatland becomes wetter.

- The process-based DOC modelling together with the distributed hydrology modelling within the framework of LPJ-GUESS WHyMe gives us the opportunity to integrate vertical (atmosphere-vegetation-soil) and horizontal (DOC routing) terrestrial carbon flows in the model, which could significantly contribute to the estimates of terrestrial ecosystem fluxes. The process-based soil DOC export and the lateral transport can potentially be linked to river and lake carbon cycling models in order to comprehensively integrate both terrestrial and aquatic carbon dynamics in a changing climate.

7. Future developments and applications

In this thesis we have shown the advantages of integrating the TFM algorithm in capturing both hydrological and ecological fluxes in the Stordalen catchment. The influences of different flow routing algorithms on ecosystem processes may differ from region to region due to climatic conditions, vegetation distribution and topographical characteristics. Thus, the benefits of the TFM algorithm in partitioning flow should be tested in a larger area. For global hydrological modelling groups, an essential required input is a global drainage map to determine flow transport directions. However, the widely used global drainage map (Döll & Lehner, 2002) was developed on the basis of a SF algorithm, which could restrict the accuracy of the estimated water flow. With the availability of global DEM data and vectorised, high resolution river maps, it is worthwhile to reproduce a global drainage map based on the TFM algorithm and test it with different global hydrological models.

To implement the cell-to-cell based flow distribution developed in this thesis in a larger catchment, an explicit consideration of flow velocity is required. The flow velocity in the current implementation in the Stordalen catchment is applied implicitly, assuming surface and subsurface water can flow out of the catchment within one time step. However, the traveling distance of lateral water (surface and subsurface) from a specific cell is dynamically determined by the soil saturation deficits of downslope grid cells and the amount of runoff from the current cell on a daily basis. With coarser resolution and a larger catchment, this assumption may not apply and the influence of flow velocity becomes more significant in determining water traveling distance within each time step. The explicit consideration of flow velocity in a larger area needs to reflect the influences of vegetation resistance, topographical characteristics as well as soil properties. However, it may be difficult to aquire and quantify such spatial information as well as validate its impacts on flow velocity in larger regions (Gong *et al.*, 2009). Moreover, for some global hydrological models, the flow generation is implemented as a linear relationship with water storage and the flow velocity is simplified as a constant (e.g. 1 m/s) for different paths of runoff (Oki & Sud, 1998, Döll *et al.*, 2003). For these models, the traveling distance of lateral water per time

step is fixed (e.g. 1 m/s equal to 86.4 km/day). If we were to apply the same constant velocity in our approach, then the maximum travelling distance of lateral runoff will be constrainted by this value. However, within the threshold value the lateral water partitioning and travel distance will still be a function of the soil saturation deficits of downslope grid cells and the amount of runoff. Therefore, our approach would be implementable for larger catchments. In addition, our current flow routing approach does not consider deep groudwater flow (baseflow) which could be developed in the future application.

In the current version of LPJ-GUESS, the water flow within the soil is still largely based on a "two-layer bucket" structure, which could be further enhanced by implementing a finer vertical discretisation to model soil water flow (Cox *et al.*, 1999, Wolf *et al.*, 2008a). By implementing finer soil layering and water flow, it may be possible to distinguish the contributions of DOC export from different soil layers (Neff & Asner, 2001).

Since the hydrological scheme is developed to fit into the framework of the dynamic vegetation model, no specific consideration of in-lake processes and potential influences from lakes on flow paths was taken. A future coupling of hydrological modelling in lakes could be considered to improve catchment water fluxes. Finally, we could also couple our terrestrial vegetation model with aquatic biogeochemical models to dynamically link terrestrial organic carbon inputs with aquatic ecosystem processes, for instance considering DOC decomposition in aquatic systems.

Finally, the current carbon budget estimations and predictions at the catchment level can be further investigated with potential N limitations on plants (Smith *et al.*, 2014). The latest version of LPJ-GUESS has coupled N cycling and C-N interactions in the model, which could be integrated into the customized Arctic version of the model implemented in this thesis.

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Avhandlingar från Institutionen för naturgeografi och ekosystemanalys (INES), Lunds universitet

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Dissertations from Department of Physical Geography and Ecosystem Science, University of Lund

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