Spatial patterns of Dissolved Organic Matter in Swedish Surface Waters

Rumslig analys av löst organiskt material i svenska vattendrag

Anna Lackner

Independent project 30 hp

Swedish University of Agricultural Sciences, SLU

Department of Aquatic Sciences and Assessment

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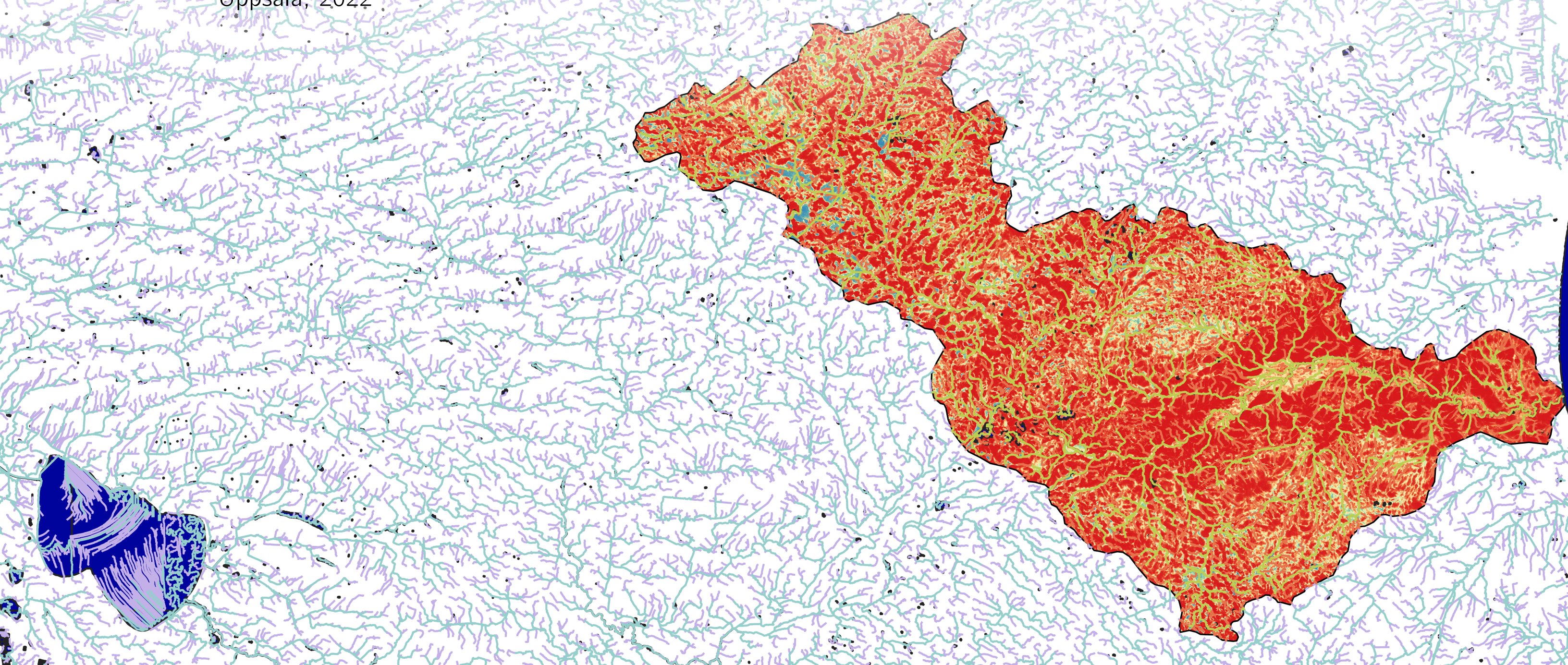

Spatial Analysis of Dissolved Organic Matter in Swedish Rivers

Anna Lackner

Supervisor	Prof. Dr. Kevin Bishop, SLU, Department of Aquatic Sciences and Assessment
Assistant Supervisor	Univ. Prof. Dr.Christine Stumpp, BOKU, Institute for Soil Physics and Rural Water Management
Examiner	Prof. Dr. Lars Lundin, SLU, Department of Aquatic Sciences and Assessment
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Swedish University of Agricultural Sciences, SLU

Faculty of Natural Resources and Agricultural Sciences (NJ)

Department of Aquatic Sciences and Assessment

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Abstract

Dissolved organic matter (DOM) in surface water has been widely studied, in part due to its significance for aquatic ecology and drinking water quality. Across Sweden, increases in the total organic carbon (TOC) concentrations and color of surface waters, known as brownification, were noted in the decades before and after year 2000, though recent analysis has found widespread DOM increase to have ceased after 2010. While the overall decadal trends of TOC have gained considerable attention, the spatial patterns in the TOC dynamics of different watercourses may hold clues to the causes of the TOC variation in time as well as in space. Recent developments in digital mapping provide high resolution information on soil moisture and the spatial variation of the extent of river systems. This thesis focused on testing whether the new, high resolution map data can explain spatial and temporal patterns in stream DOM. In addition to the soil moisture map, modeled stream networks were used to more accurately represent the small streams of the headwaters, and locate hydrological connectivity of soils near streams. Data taken from the soil moisture map and modeled stream networks were used as high resolution data in the analysis. In changing the stream initiation size of the modeled streams from 10 ha to a smaller area needed for stream initiation of 2 ha the stream systems length in Sweden showed a mean increase by 41% while increasing stream initiation size to 30ha decreased the stream network length by 46%. Adding high resolution data did not improve the ability of the multivariant model to explain TOC variation and influences that already included catchment characteristics such as meteorological, discharge, soil type and land use data, which could explain 64% of variation. However, on its own high resolution data was able to explain 40% of the variation in TOC and its influences. In conclusion high resolution spatial data of soil moisture and stream length although they could not add new explanatory power, can be used to deepen our understanding of the importance of topographic variables to TOC variation.

Popular-scientific summary

In the late 20th century a darkening in the color of boreal waterways including Sweden was observed sparking research interest. The phenomenon was termed as brownification and was due to an increase in dissolved organic matter and iron concentrations. Changes in dissolved organic matter of surface waters can impact the aquatic community as water quality changes, and complicates the use of surface water for drinking water. Initial brownification trends have been linked to acid decomposition though factors such as climate, weather, as well as catchment characteristics such as land use and type also impact dissolved organic matter concentrations. Dissolved organic matter concentrations were predicted to continue increasing into the 21st century. However, a recent study has found that brownification has halted in most catchments across Sweden. A previous study divided catchments changes in dissolved organic matter throughout the year up into changes dependent on the seasonality, flow, and consistent long term changes. Dissolved organic matter behaviour in terms of long term brownification as well as seasonal changes varies from catchment to catchment. Another previous study divided catchments changes in dissolved organic matter throughout the year up into changes dependent on the seasonality, flow, and consistent long term changes. The goal of this thesis was to find the differences in the catchment characteristics that could explain the difference in dissolved organic matter behavior previously identified. Specifically, the ability of a Sweden wide high resolution digital map of soil moisture to explain the different dissolved organic matter behaviour previously observed for 215 catchments in Sweden. Wetter areas are known to be major contributors of organic matter. Additionally, areas adjacent to the stream are known to be the major source of organic matter. Therefore, the digital map was used to extract information of soil moisture near streams and for the entire catchment, and used to statistically explain differences in dissolved organics matter behaviour for 215 Swedish catchments.

It was found that high resolution soil moisture information was unable to improve the ability of traditionally used catchment characteristics to explain differences in dissolved organic matter behaviour. Although the high resolution data did not improve the ability to explain dissolved organic behaviour it was able to emphasize the importance of mesic moist areas and lakes in the catchment and the dissolved organic matter processes associated with these characteristics. Further the results steer attention for further research to the characteristics not considered by this study. Additionally, this thesis was able to extract data at a large scale and high resolution with limited computing power, demonstrating the potential of the use of digital maps when answering questions at a high resolution and nation wide scale.

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List of Abbreviations

DEM	Digital Elevation Model
DOC	Dissolved Organic Carbon
DOM	Dissolved Organic Matter
LiDAR	Light Detection and Ranging
OM	Organic Matter
PCA	Principal Component Analysis
PLS	Partial Least Square Regression
PPM	Parameter Parsimonious Model
SMM	Soil Moisture Map
SMC	Soil Moisture Cover
TA	Trend Analysis
TOC	Total Organic Carbon
VIP	Variable Importance in Projection

1 Introduction

1.1 The Question of Brownification

Towards the end of the 20th Century increases of organic matter in surface waters across North America and Europe were observed as changes in total organic carbon (TOC) and changes in the water color (Driscoll et al. 2003; Wit et al. 2007; Erlandsson et al. 2008). As surface water increased in OM and iron, they brownified, darkening in surface color. The start of widespread brownification in Sweden occurred in the 1970s and continued to be observed into the early 2000s (Erlandsson et al. 2008). Although browning was expected to continue (Wit et al. 2016; Kritzberg 2017), a recent study by Eklöf et al. (2021) found that brownification in Swedish catchments may have ceased or halted since 2010. It was shown that when using long term monitoring data of the past 30 years a clear pattern can be seen where brownification occurred widespread across Sweden before 2010, but after 2010 browning no longer occurs as wide-spread. Previous studies had found brownification to be most dramatic in the boreal regions, such as Sweden (Björnerås et al. 2017), likely due to the extensive carbon pool in the boreal region which stores at least 1/3 of the terrestrial carbon (Bradshaw and Warkentin 2015). Although brownification, its causes, and consequences have been studied extensively since its first observations in the sixties, studies have focused on using large scale monitoring data or small scale catchment studies to understand the processes involved and carry out assessments. Trend analysis has taken different forms from long term analysis such as Eklöf et al. (2021) to using modeling in order to understand the processes and influences controlling DOM such as Monteith et al. (2007) and Hytteborn et al. (2015). The data available for such analysis is usually taken from monitoring networks and consequently is an account of what happens at the outlet of a catchment. As Bishop et al. (2008) argues there is a lack of studies about what happens in the headwaters, even though the headwaters are an essential part of the river network. The headwaters make up a significant portion of the land water interface (Meerveld et al. 2020). The land closest to the stream, the riparian zone, has been found to have substantially greater DOC concentration compared to soils further from the stream (Lidman et al. 2017). Consequently, headwater streams and their nearby soils are of importance to DOC export (Ledesma et al. 2018).

River networks have traditionally been mapped as stationary systems, however, river systems can expand and contract in time changing in length (Bishop et al. 2008; Benstead and Leigh 2012). Traditional maps have missed not only mapping intermittent streams but also small streams and channels of the headwaters. Ågren et al. (2015) found that current maps missed 58% of the perennial stream network and 76% of the fully expanded stream system. Trend analysis such as Eklöf et al. (2021) and the break down of trends into its influences through a parameter parsimonious model as done by Hytteborn et al. (2015) can further the understanding of DOC patterns, while looking in the headwaters may be able to explain the variation of these patterns. Therefore, to understand DOM and the changes that will occur in the future it may be necessary to connect information from the headwaters to trend analysis at the outlet. The lack of information used to study DOC in the headwaters is largely due to the lack of available information as sampling low-ordered stream would be extensive work that is not commonly done unless a specific small scale study is carried out. However, modern advances in technology such as high resolution remote sensing and machine learning have high potential to fill in knowledge gaps concerning the headwaters. High resolution mapping can be used to extract information about the stream extent, the riparian zone and the catchment as a whole. In using high resolution data of the headwaters trend analysis can be understood as a function of the characteristics of the headwaters.

1.2 Dissolved Organic Matter

Organic matter (OM) in water is split into two categories: particulate organic matter and dissolved organic matter, which can be distinguished through filtration. Dissolved organic matter is made up of roughly 50% carbon, so even though dissolved organic carbon is not equal to dissolved organic matter, for the purpose of the discussion of trends and patterns in this study the two terms are used interchangeably. As in Sweden several studies have found DOC and TOC to have a difference of only a few percent, TOC analysis is taken to represent DOC behaviour (S. Köhler 1999; Laudon et al. 2011).

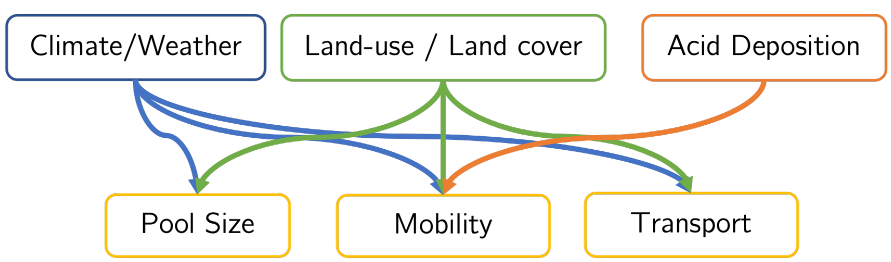

Fig. 1: Climate/Weather, Land-use/ land-cover, and Acid Deposition control the export of DOM in the catchment by determining the pool size, mobility and transport of OM to the stream. Adapted from Kritzberg et al. (2020).

1.2.1 Consequences

DOC export in Swedish waterways is a significant component of the carbon cycle from a major pool of global terrestrial carbon (Laudon et al. 2004) and has the potential to effect the global carbon cycle. DOC also influences other biochemical substances by acting as a carrier. For example, DOC influences the speciation, mobility and bioavailability of mercury and other cationic metals (Lydersen et al. 2002). In waters with higher DOC concentrations, higher mercury concentrations have been found in fish and invertebrates (Creed et al. 2018). However, dissolved organic matter is not only important for the biochemistry of the waters, but plays an important role in the ecosystem services provided by surface waters. Surface water can be used as a drinking water supply. In Sweden 75% of the drinking water supply is potentially affected by DOC changes in surface water, as it is sourced from surface waters (50%) or artificial infiltration of surface waters (25%) (Kritzberg et al. 2020). Although there is no legal limit on DOM in Swedish drinking water there is a recommendation of 4 mg/L (S. J. Köhler et al. 2016). Increases in DOC increase cost of the chemical used to precipitate DOC or if DOC is too high it can prompt the need for high cost modern filter technology such as nano-filters. DOC in drinking water supply can interfere with other treatment processes such as activated carbon filtering, further complicating drinking water treatment (Kritzberg et al. 2020). Brownification of surface water can have negative impacts on the recreational service of the water as clear water is preferred for recreational use over brown waters (Hadwen and Arthington 2003; Keeler et al. 2015).

1.2.2 Factors

DOC concentrations in surface waters are determined by the initial pool size, the mobility of OM and the transport to and in the river system. The carbon pool size is governed by biomass production and decomposition. A larger carbon pool size relates to a greater export of DOC (Weyhenmeyer et al. 2014). Mobility of DOC is governed by biochemical factors such as pH, Redox, and ionic strength. The transport of DOC is governed by the hydraulic connectivity as well as the hydrology and precipitation of the catchment. Changes in DOC have been attributed to different factors that can impact these three determinants, most importantly atmospheric deposition, land cover and land use changes, and climate change. The recovery from acidification through atmospheric deposition of sulfate in the second part of the 20^{th} century led to an increase of the mobility of OM (Monteith et al. 2007). As OM had acted as a buffer for the acidity of the system during years of high sulfate deposition, once sulfate deposition decreased DOC concentrations increased again. Climatic factors can influence the carbon pool size, mobility and transport of a system, by affecting biomass production, decomposition rates, pH, and hydraulic connectivity. Precipitation is responsible for runoff, connecting the catchment carbon pool, and it can also raise the water table and thereby increase hydraulic connectivity between organic soils and surface waters (Laudon et al. 2011). Precipitation changes in turn can change the spatial extend of the river system, and therefore the extent and make up of the riparian zone (RZ). The RZ is a major contributor of OM; with TOC concentrations higher by up to 10 times in the riparian zone compared to mineral soils further from the stream (Lidberg et al. 2017). Increasing temperatures stimulate decomposition of OM and biomass production, affecting both carbon pool and mobility (Larsen et al. 2011; Finstad et al. 2016). Similarly, land cover and land use influence all three determinants. Long term DOC data of southern Sweden suggests that afforestation has had a major role in brownification, but that since build up of carbon pools is slow there is a lag of several decades (Kritzberg 2017). Land use management methods such as clear cutting have also been found to increase short term DOC fluxes, by mobilizing DOC (Schelker et al. 2012).

1.2.3 Trends and Patterns

Increasing brownification prior to 2000 has been attributed largely to a decrease in atmospheric sulfur deposition (Monteith et al. 2007). Sulfur emissions decreased in Europe by 70% since 1990, while from 2015 onwards, a further decrease of 10% was projected (Maas and Greenfeldt 2016). Instead of sulfur deposition as main driver, changes to a wetter climate (Wit et al. 2016) and afforestation (Škerlep et al. 2020) were reasoned to continue driving brownification in the future. To check whether this continuing brownification trend was occurring as predicted Eklöf et al. (2021) used extensive records of TOC data from the Swedish monitoring system. They quantified TOC trends from before and after 2010, finding a reduction of brownification trends (Figure 2). This contrast between predicted trends and observed trends in DOM prompts the need to question the known drivers of DOM. Since management decisions are based on predictions understanding the drivers of DOM is essential for making predictions as well as management decisions.

TOC trends are neither monotonic in time nor space (Eklöf et al. 2021). While Eklöf et al. (2021) quantified the temporal changes in TOC trends, Hytteborn et al. (2015) used monitoring TOC data to systematically quantify the effects of different drivers on TOC (Figure 3). In explaining TOC patterns using influences of long term trends, seasonality, and discharge for 215 different catchments in Sweden, Hytteborn et al. (2015) was able to characterize each of these catchments according to their influences of

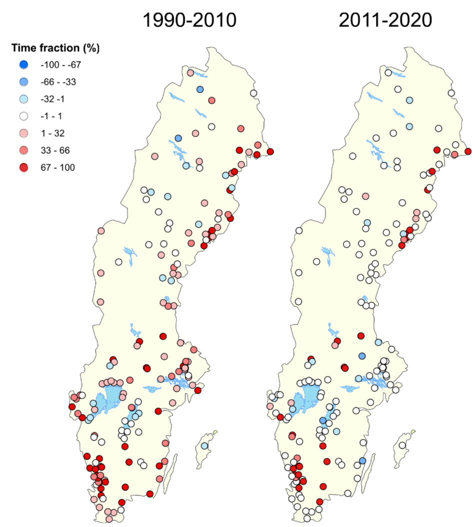

Fig. 2: Time fractions (%) of significant TOC trends for the periods 1990-2010 and 2011-2020. Increasing trends are colored in red, decreasing trends in blue, while white denominates no trend. Trends had been determined for each month of the period in order to calculate the time fraction for the whole period. Opposing trends for different months within the same time period, canceled each other out to be neutral. Taken from Eklöf et al. (2021).

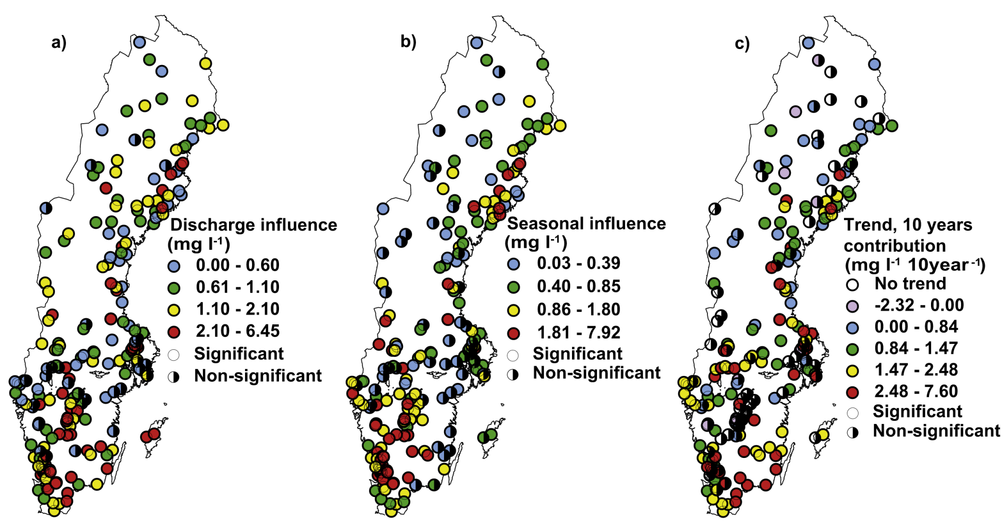

Fig. 3: Influences of (a) discharge, (b) seasonality and (c) trend on TOC variability. Color ranges from blue to red are based on the 1st, 2nd and 3rd quartiles for each influence. Taken from Hytteborn et al. (2015).

TOC. In using results from Eklöf et al. (2021) and Hytteborn et al. (2015) TOC behaviour for a selection of catchments with TOC, monitoring data can be characterized in both their patterns as influenced by seasonality, flow, and trend as well as long term changes in trend, all of which are independent characteristics of each catchment.

1.3 High Resolution Digital Mapping

Since digital mapping emerged in the middle of the 20th century its availability, usage, and wealth of information has expanded drastically through the development and expansion of new remote sensing techniques, computing power, and storage capacity. Topographic maps were originally made using field observations. Nowadays most topographic maps are drawn from aerial photographs, while light detection and ranging (LiDAR) campaigns are starting to be more widespread on a national scale. With each of these advances, topographic mapping has become more efficient with a higher resolution. LiDAR has several advantages as it can detect the ground underneath the canopy and produce a digital elevation model (DEM) with a 2m resolution at high accuracy (Kanostrevac et al. 2019). In contrast aerial photographs are limited by the canopy cover and are unable to give information about what happens underneath the canopy.

Within Sweden advances in high resolution digital mapping have been motivated by their usage within planning forestry operations. Heavy machinery used in forestry operations can cause rutting and soil compaction (Naghdi and Solgi 2014), which in turn affects the soil biology (Frey et al. 2009), gas emissions from soil (Teepe et al. 2004), and forest growth (Curzon et al. 2014). Additionally, rutting has been found to lead to increased mercury export to surface waters (Eklöf et al. 2015). Digital maps in forestry can be used to minimize negative impacts on the environment by informing on the location of small streams and wet areas that are most vulnerable to rutting and soil compaction. Currently depth to water maps calculated from DEM are used for determining wet areas in Swedish forestry for planning. To improve the ability of predicting wet areas and minimize forestry impacts, new digital maps using high resolution LiDAR generated DEMs and machine learning to predict wet areas (Lidberg et al. 2020) and soil moisture (Ågren et al. 2021) have been developed. Although these maps were motivated by improving forestry operation planning, they are a large scale source of information at a high resolution which can be used to characterize catchments at a greater resolution than most other digital maps available. Soil cover and land use cover of Sweden is available at a resolution of 25-1000m while the soil moisture map (SMM) by Ågren et al. (2021) has a resolution of 2m. The riparian zone has been found play a major role in the export of DOC (Lidman et al. 2017) suggesting that the area closest to the stream may be most relevant to DOC concentrations in the stream. If the area close to the river is relevant, high resolution SMM may be able to provide information catchment analysis using traditional ancillary data may have missed.

1.4 Objectives

Catchments in the boreal region typically have a organic rich histosols near streams and mineral podzols upslope (Ledesma et al. 2018). These organic rich soils near stream are a result of paludification in consequence of long term interaction of landscape, climate, biota and disturbances (Lavoie et al. 2005). The accumulation of carbon in the RZ may be explained by the combination of high productivity due to high nutrient availability (Jansson et al. 2007) and limited degradation due high groundwater tables creating anoxic conditions (Luke et al. 2007). This suggests that areas with greater soil moisture store more carbon. The importance of soil moisture to carbon stocks is further supported by a soil moisture being the key covariate for predicting soil carbon stocks in Sweden (Hounkpatin et al. 2020). The DOC quality and quantity in the RZ have been found to match in stream DOC, suggesting the main source of DOC to be in the RZ (Ledesma et al. 2015). RZ width has in turn has been found to explain about 90% of DOC fluxes in a headwater catchment in northern Sweden (Ledesma et al. 2015). RZ width is spatially variable and based on field observation, Ledesma et al. (2015) found RZ between 2-93m wide. Based on the importance of the width of the RZ and the characterization of the RZ as near stream areas with high soil moisture content associated with a high groundwater table, determining the soil moisture cover[1] (SMC) near stream can indicate variation in the RZ, and therefore DOC export. It is therefore expected that the soil moisture cover near the stream is of more importance in explaining DOC variation than the soil moisture cover for the entire catchment. Furthermore, as the stream network extents in length at high flow, more area is connected and may become part of the RZ contributing to DOC export. In considering the soil moisture cover of the area connected to the RZ during periods of lengthened river systems, the changes in the carbon pool hydrological connected to the stream can be identified. When considering the influences on DOC as described by the parameter parsimonious model of Hytteborn et al. (2015) catchments in which DOC flux is influenced by discharge are experiencing greater DOC during periods of an expanded stream system. Assuming that the increase in DOC comes

[1] Soil moisture cover, or SMC, refers to the spatial distribution of the different soil moisture categories as used in the machine learning soil moisture map, SMM, of Sweden published by Ågren et al. (2021).

from the added carbon pool along the expanded streams, catchments that add more area with greater soil moisture near the stream with an expanding system are hypothesized to have a greater influence of flow on DOC. Due to the compacted till soils of Sweden and the associated exponential reduction of hydraulic conductivity along the soil profile subsurface flow occurs mostly in the top 30 cm (Bishop et al. 2011), leading to the assumption that subsurface flow follows surface topography, one of the key assumption for using distance to stream by flow-path instead of euclidean distance and the topographically modeled stream systems. This is an assumption that is only appropriate for Sweden and not areas with different hydrological conditions.

By combining the DOC information found in large scale trend analysis and high resolution digital mapping data of stream extent and soil moisture content, we see the potential to connect what goes on in the headwaters with DOC behaviour further downstream where water chemistry is monitored. This study therefore aims to explain trend analysis of TOC through high resolution spatial data of soil moisture and stream extent. Thus, the thesis had these objectives:

- Calculating stream lengths for stream systems modeled using different stream initiation sizes.
- Extract soil moisture cover near stream and for the entire catchment from the SMM.
- Statistically test whether extracted high resolution information could explain the spatial variation of trend analysis results from Eklöf et al. (2021) and Hytteborn et al. (2015).

2 Material & Methods

High resolution soil moisture cover along the river system and for the whole catchment were extracted by geo-spatial programming from the machine learning soil moisture map (SMM) published by Ågren et al. (2021) for 215 catchments across Sweden. Stream length and density were calculated from modelled stream networks using three different stream initiation sizes: 2ha, 10ha, 30ha. Two different trend analysis were used to represent DOM trend variability across Swedish catchments: a long term DOM trend analysis which showed how trends have evolved in the period from 1990 to 2020 (Eklöf et al. 2021), and a parameter parsimonious model of DOC before 2010 consisting of the trend, seasonal and discharge influences on DOC (Hytteborn et al. 2015). In order to investigate the connection between soil moisture and DOM trends for these catchments a multivariate analysis was performed using the extracted high resolution data (soil moisture cover and stream length), and traditional data (90 additional catchment characteristics including land use, soil type, and meteorological data) to explain the spatial variation in DOM trend analysis.

2.1 Study Area

The data used for this study spreads across the northern European country of Sweden. Sweden lies within 55-70°N and 11-25°E. Sweden has a mean annual temperature ranging from 8°C in the south to -2°C in the north (Seekell et al. 2014). For the catchment based analysis 215 Swedish catchments are used ranging in size from 0.18 km^2 to 30 640 km^2 with an average catchment elevation between 22 to 957 meters above sea level. As Sweden has been through several periods of glaciation in the past 2-3 million years, about 75% is covered in glacial till left behind after the last glaciation 22 000 - 10 000 years ago (Fransson 2018). After glacial till, peat is the second most dominant soil type at 13% (Fransson 2018). As published by the Swedish Land Cover Database Sweden's land cover consists of 63% forest, 8.9% lakes, 8.7% open mires, 7.7% heathlands, 6.1% arable land, 2.8% forested mires, 2.3% urban area, and 0.6% other (Ansén 2004).

2.2 Trend Data

2.2.1 Long-term trend changes

Eklöf et al. (2021) investigated the long term trends of OM in Swedish waterways by looking at TOC sampled at 164 watersheds between the period of 1990 and 2020. Consecutive sampling periods for the

164 watersheds used, averaged a length of 27 years of sampling mostly monthly (n=117), some twice a month (n= 37), and some bimonthly (n=10). In order to identify patterns in temporal changes in organic matter Eklöf et al. (2021) used generalized additive mixed models, as this approach allows for trend analysis without prior definition of the shape of the trend. The results showed an increase in TOC concentrations for a majority of the sites in the period prior to 2010, though these were neither linear nor monotonic. After 2010 only 20% of the sites showed a significant increasing trend in TOC, suggesting that browning of Swedish waterways has largely ceased or is 'on-hold'. For each catchment time fractions were calculated for both periods (1990-2010 & 2011-2020) representing the percentage of the time period the catchment had a negative or positive trend or no trend at all. A positive time fraction refers to an increasing trend while a negative trend is represented by a negative time fraction. A spatial analysis was beyond the scope of the study by Eklöf et al. (2021).

2.2.2 Parsimonious model of TOC trend

Hytteborn et al. (2015) investigated inter-annual and intra-annual variation of DOC by systematically quantifying the effects of discharge, seasonality and trend on TOC concentrations of 215 catchments in Sweden. This was done using a parameter parsimonious model with TOC calculated as:

$$TOC = e^{a_0} * Discharge^{a_1} * e^{A*sin(2pi*dtime+c)} * e^{a_4*dtime} \tag{1}$$

The parameter parsimonious model consists of four terms a constant term (e^{a_0}), a discharge term ($Discharge^{a_1}$), a seasonality term ($e^{A*sin(2\pi*dtime+c}$), and a trend term ($e^{a_4*dtime}$), where a_1 is the discharge coefficient and a_4 is the trend coefficient. The seasonality term is more complex with two coefficients: A, the amplitude and c, the displacement. While A gives the magnitude of the seasonality term c determines when the seasonality has its highest value. Hytteborn et al. (2015) used TOC data from the Swedish monitoring system (Fölster et al. 2014) with each watershed having at least 6-years of monthly data in the 21-year period from 1990 to 2010. The Fluxmaster software package (Schwarz et al. 2006) was used as a statistically optimized framework to estimate daily TOC concentrations and loads for use in Equation 1 based on long term monitoring data. Hytteborn et al. (2015) was able to fit models with significant discharge and trend coefficients for 149 of the 215 catchments. TOC variation investigation also showed that intra-annual TOC variation exceeded inter-annual variation. Hytteborn et al. (2015) performed PLS analysis to see what variables could explain the variation in parameter parsimonious model coefficients and performance based on discharge, average area and elevation for the catchment (50m resolution), land use (100m resolution), soil type (25-500m resolution), forest geographical data, precipitation and temperature, modeled retention time, modeled carbon and nitrite content in soil (Table S2). For the purpose of this thesis these data are used as "traditional" data in comparison to the high resolution data extracted within this work, and will be referred to as such.

2.3 Spatial Data

Ågren et al. (2021) used LiDAR-derived terrain indices and machine learning to generate a high resolution soil moisture map (SMM) across the Swedish forest landscape. LiDAR data from the Swedish Mapping, Cadastral, and Land Registration Authority was used in the form of a digital elevation model (DEM) with a grid resolution of 2m (Lidberg et al. 2020) for the calculation of terrain indices. DEM calculated indices were complemented by maps of ancillary environmental variables to adjust for local and regional conditions. Ancillary maps used include Quaternary deposits, and soil depth from the Swedish Geological Survey, as well as modeled discharge from the Swedish Meteorological and Hydrological Institute. In addition soil moisture data from 19,643 National Forestry Inventory plots were used to train and test the SMM. Five machine learning mechanisms were tested and evaluated for generating categorized and continuous soil moisture maps. The machine learning algorithm XGBoost was used to calculate the probability for each pixel to be wet. This resulted in a continuous soil moisture map at a resolution of 2m grid cells which was released as an open geo-data map for all of Sweden (www.slu.se/mfk).

In the process of creating machine learning wet area maps of Sweden Lidberg et al. (2020) generated digital maps of streams at different stream initiation sizes between 0.5 and 30 ha. Stream initiation sizes, also referred to as 'source areas' set the threshold the drainage area needed before the stream is initiated. Ågren et al. (2015) found for a 68 km^2 forested catchment in northern Sweden, a 10 ha stream initiation size to represent base flow. Although this will vary depending on the specific catchment, a stream initiation size of 2ha, 10ha, and 30ha, were used for this study to roughly represent high flow, base flow, and low flow conditions (Figure 4). The modeled stream systems split into 2 818 sub-catchments are available as open geodata from the Swedish Forest Agency, Skogsstyrelsens (www.skogsstyrelsen.se). The same LiDAR data and DEM as for the SMM map was used for the generation of the stream networks. The three diffrent stream networks were used for calculations of stream length and soil moisture extraction near rivers. The DEM used for the modeling of the streams and the creation of the soil moisture map had been pre-processed by breaching as described by Lidberg et al. (2017).

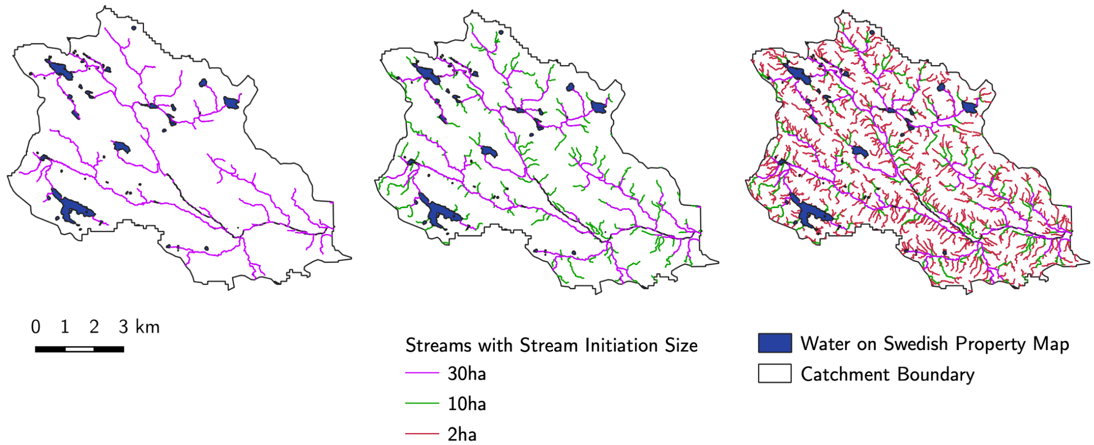

Fig. 4: Spatial dynamics of a stream network: As the stream initiation size decreases and the river moves from low flow conditions to high flow conditions the stream network expands and lengthens. A stream initiation size of 2ha represents high flow conditions, a stream initiation size of 10 ha represents base flow, and a stream initiation size of 30 ha represents low flow conditions.

2.4 Geospatial Extraction

2.4.1 Soil Moisture Extraction

For each catchment soil moisture cover for the whole catchment, within 10m meters of the stream measured in flow path distance and within 100m were extracted from the soil moisture map for three river systems with stream initiation sizes of 2ha, 10ha, and 30ha. As the digital maps used take up significant storage space and processing power data extraction methods used tried to minimize the need for computing power while retaining information contained within the maps. This was done by dividing the available data in 2 818 sub-catchments and automatizing the processing by looping through each sub-catchment within a Python script. Open source libraries including gdal, geopandas, and whitebox tools, as well as arcpy, the geospatial library from the professional GIS program ArcGIS, were used for the processing of the data. For each sub-catchment LiDAR derived DEMs preprocessed by methods described in Lidberg et al. (2017) were used to calculate the flow path distance to stream (FDS). In order to avoid edge effect each of the DEMs and FDSs used had a 2 km overlap with adjacent sub-catchments. To extract only data within the boundaries of the catchment rasters of matching extent, cell size and alignment were generated for each catchment denominating each cell as within the catchment or outside. Similarly, for each sub-catchment rasters with matching extent, cell size and cell alignment to the FDSs were cut out from the SMM. Once the three rasters were produced for each catchment they were read into flattened NumPy arrays (a python and R compatible array format). They are essentially a point cloud of the raster data without spatial reference, with each value in the array referring to a matching cell for the three rasters. By overlaying the information of each of the three arrays, as shown in Figure 5, the number of pixels for five different soil moisture classes were extracted. This was done three times: for the whole catchment, for FDS less than 10 and for cells FDS less than 100. The two different FDS sizes were extracted 3 times for the three different stream initiation sizes. The SMM map values ranging between 0-101 representing the probability of being wet, were categorized into 6 classes: dry (0-4), mesic (5-37), mesic-moist (38-91), moist (92-98), wet (99-100), and lakes (101). The five moisture classes used were defined based on Ågren et al. (2014): "wet" soils are organic with a high ground water table that leads to permanent water standing on soil surface. "Moist" soils are organic (fens) or mineral soils (humus-podsols) with a water table averaging less than 1m depth, dominated by wetland mosses in depressions while trees showing coarse root system above ground. "Mesic-moist" soils are humoferric to humic podsols with mineral soils covered by a thick layer of peat, which have a groundwater table above 1 m depth covered and are covered in wetland mosses. "Mesic" soils have a groundwater table at 1-2m depth and a distinct bleached white-grey horizon in comparison to the rust-yellow/brown/red B-horizon, and are covered in dryland mosses. "Dry" soils have a groundwater table below 2m depth and form on heightened terrein features such as eskers, hills, and ridges. They tend to have coarse soil and may have significant exposed bedrock.

The pixel count for each sub-catchment was collated for each of the original 215 catchments. For this a dictionary had been created that linked the 215 catchments to the sub-catchments that are contained within. As some catchments (n= 88) were smaller than the sub-catchments, the whole process was repeated using a raster categorizing cells as within the catchment rather than within the sub-catchment. From the summed up pixel data for each catchment the difference in soil moisture cover for the different distances used were calculated by the equation:

$$\Delta_{xha} = \frac{soil_{10ha} - soil_{xha}}{tot_{10ha} - tot_{xha}} \tag{2}$$

where Δ_{xha} is the change in the specified soil moisture type between x and 10ha and *soil* is the pixel count for the soil moisture type, and tot is the total pixel count.

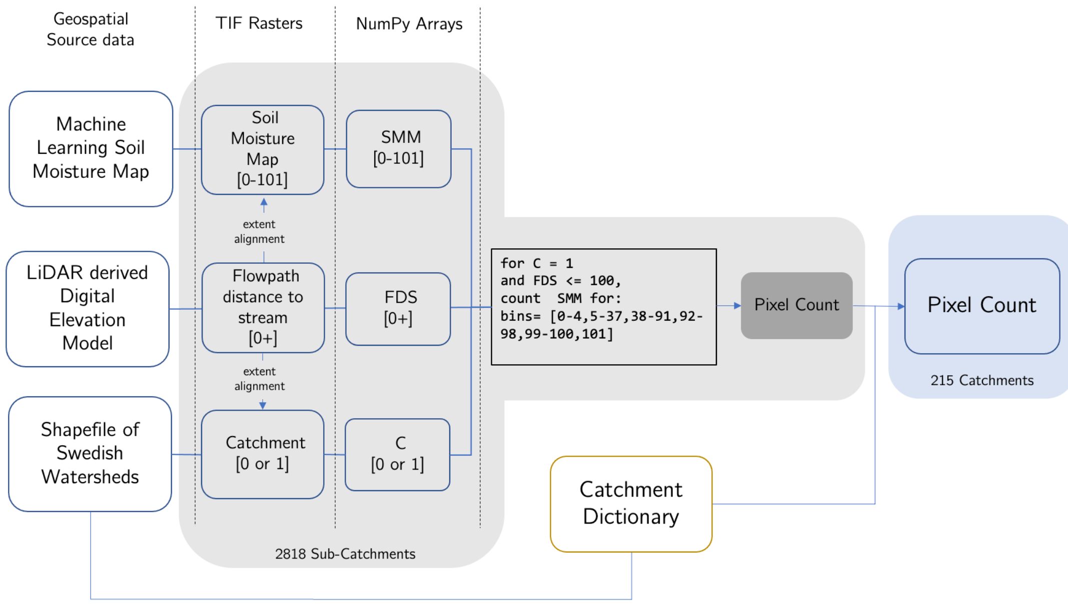

Fig. 5: Schematic diagram of the procedure used to extract soil moisture content from high resolution digital maps. For more details on the creation of the Catchment Dictionary see Figure S1.

2.4.2 Stream Length Calculation

In order to quantify the changes of the length of the stream systems for the different initiation sizes, stream lengths were calculated. The open source stream data was pre-processed by merging the 2 818 sub-catchments to a Sweden wide network and subtracting open waters from the Swedish property map from the stream network. As the stream networks had been generated using LiDAR data open water can generate noise within the data that shows up as a high density line system spread across the surface of the open water (Figure S2a). The open waters of the Swedish property map serve to eliminate these extra lines within the stream network, however, as they do not match exactly remnants of the lines were left to be included in the stream length calculations (Figure S2b). From the remaining stream network the length of the streams for the three initiation sizes were calculated, as well as the change in stream length from the 10 ha stream initiation size.

2.5 Statistical Analysis

Before multi variant analysis relating the extracted variables to DOM trends the data was visually inspected for non linearity and possible miss-calculations in the geo-spatial extraction. Catchments which had less than 50% covered by the soil moisture map were removed from further analysis. For further analysis if missing data existed for a catchment it was excluded from the analysis. Principal component analysis was performed on the high resolution data to explore the relation of the extracted variables to one another for 208 catchments. For the statistical relationship testing of trend data with the high resolution data catchments which did not have a significant parameter parsimonious model, or a time fraction to compare to were removed from the multi-variant analysis. As soil moisture cover is given as a percentage and all the categories add to 100 it is compositional data and had to be transformed before it can be used in multi variant analysis (Aitchison 1983). A log-ratio transformation was therefore applied:

$$soil_{transformed} = log(\frac{soil}{soil_{mesic}}) \tag{3}$$

where soil is the soil moisture type considered originally extracted as the percentage of the total area considered and $soil_{mesic}$ is the percentage of mesic soil moisture cover for the same area. Since the last component does not add any additional information for modelling purposes it does not matter statistically which component is chosen as the denominator of the ratio. Since all other categories had values of zero in at least one catchment considered the mesic soil moisture type was chosen as the denominator of the log ratio for compositional data. It is not apparent whether Hytteborn et al. (2015) included the transformation of compositional data in the original spatial analysis of the parameter parsimonious model results, however, it is a key step in the statistical analysis of this thesis. Furthermore, the logarithm of stream density variables was used as stream density showed a more normal distribution when transformed by the logarithm.

Principal component analysis (PCA) was used to investigate the relationship between extracted variables. PCA is a dimension reduction method which creates a new set of variables which are linear combinations of the original variables capturing the most information from the original variables while being statistically independent (Wold et al. 1987). The principal components determined by PCA can therefore be used to show which variables linearly relate to one another. In order to simplify the visual representation the loadings for the 62 high resolution variables found in the PCA were divided into five clusters using kmean clustering. To test for statistical differences between distance to stream used, paired t-tests were performed for each transformed soil moisture type at a stream initiation size of 10ha. For the multi-variant analysis projection to latent structure regression (PLS), also known as partial least square regression was used due to its capacity to deal with variables that are co-linearly related. (Aitchison 1983). For PLS analysis 32 of the original 62 high resolution variables were used. Preprocessing of data

Table 1: Response (Y) variables and predictive (x) variables used for multi variant analysis. For each DOC analysis considered PPM (Hytteborn et al. 2015) and TA (Eklöf et al. 2021) three PLS models were used: one using high resolution data as x-variables, one traditional resolution data as x-variables, and one using both high resolution and traditional data as x-variables. Where available basic statistics of the variables were used, i.e. mean, median, max, min, standard deviation, and coefficient of variance

Response		**Explanatory Variables**	
PPM	TC	Traditional	High Resolution
TOCm	TOCm	Area	$\text{SMC}_{\text{catchment}}$
TOC_{P25}	TOC	Elevation	Δ $\text{SMC}_{\text{2-10ha, 10-30ha; 10m, 100m}}$
TOC_{P75}	Δ Time Fraction	Discharge	$\text{SMC}_{\text{2ha, 10ha, 30ha; 10m, 100m}}$
Discharge Coefficient		Spec. Discharge	$\text{Stream Length}_{\text{2ha, 10ha, 30ha}}$
Amplitude		Soil Cover	Δ $\text{Length}_{\text{2-10ha, 10-30ha}}$
Trend Coefficient		Land Use	Δ $\text{Length}_{\text{2-10ha, 10-30ha}}$
		Tree Volume	Area
		C:N Ratio	Elevation
		Temperature	
		Precipitation	

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was done in Python using the geopandas library while JMP 16 and R was used for statistical methods.

A total of 6 PLS models were fitted: for each trend analysis one PLS was fitted using only traditional ancillary catchment data and low resolution spatial data as predictor variables, one using only the extracted high resolution data as predictor variables, and one using both traditional and the extracted data. Table 1 shows the predictor and response variables used for each PLS. For each PLS model the amount of variation of the response variables the model can explain and the efficiency of the model based on K-fold validation with 10 folds were calculated, R^2 and Q^2, respectively. Because PLS does not give the relative significance of each variable, Variable Influence on Projection (VIP) scores were calculated for each explanatory variable (Eriksson et al. 1995). The greater the VIP score the more important the variable is for explaining the variation of the response. The cutoff for what VIP score is considered important changes depending on the data set, however, generally a VIP score above 1.0 refers to important variables while a VIP score below 0.8 is understood as having limited importance (Eriksson et al. 1995).

3 Results

3.1 Stream Length

Fig. 2 shows the length and changes in length of the river system extent for Sweden, for modeled stream systems not included in the Swedish soil property map. When decreasing the initiation size from 30ha to 2ha the stream system expands by 3.5 times, from $8.15\text{x}10^5$ km to $2.87\text{x}10^6$ km. Average stream density increases 1.8 fold when changing from a stream initiation size of 30 ha to 10 ha, and another 2.9 times when reducing the stream initiation size further to 2ha.

Table 2: Results of stream length calculations, performed for stream initiation sizes of 2ha, 10ha and 30ha.

Initiation Sizes	2ha	10ha	30ha
Total Length in Sweden	$2.87\text{x}10^6$ km	$1.3\text{x}10^6$ km	$0.815\text{x}10^6$ km
Average Stream Density	9.26 km^{-1}	3.19 km^{-1}	1.75 km^{-1}
Mean change in Stream Length from 10 to 30ha		$-46\%[-43,-48]$	
Mean change in Stream Length from 10 to 2ha		$+141\%[[123,151]$	

3.2 Soil Moisture Cover

The mean SMC near streams decreases for soil type mesic-moist, moist, and wet increasing the distance from the stream considered from 10m to 100m to the entire catchment. The greatest difference occurs for the mesic moist soil type as mean SMC changes from 44.2% within 10m of the stream by flowpath distance to 35.0% within 100m of the stream and further to 27.7% when considering the whole catchment (Table 3). SMC of dry and mesic soil moisture types increase when considering more area further away from the stream. With the exception of the dry soil moisture type variation of SMC among catchments is greater in the area within 10m of the stream compared to 100m and the entire catchment (Figure 6). Paired t-tests between 10m and 100m near near stream for a 10ha stream initiation size found significant difference for each soil moisture type with $p<0.00$.

Table 3: Table of mean SMC type for stream initiation size of 10ha for area with a flow path distance to stream less than or equal to 10 m and 100m as well as the whole cacthment.

	dry	mesic	mesic-moist	moist	wet	lakes & others
10m	0.005	0.079	0.442	0.164	0.105	0.183
100m	0.119	0.218	0.350	0.101	0.103	0.108
Catch.	0.264	0.326	0.277	0.064	0.070	0.054

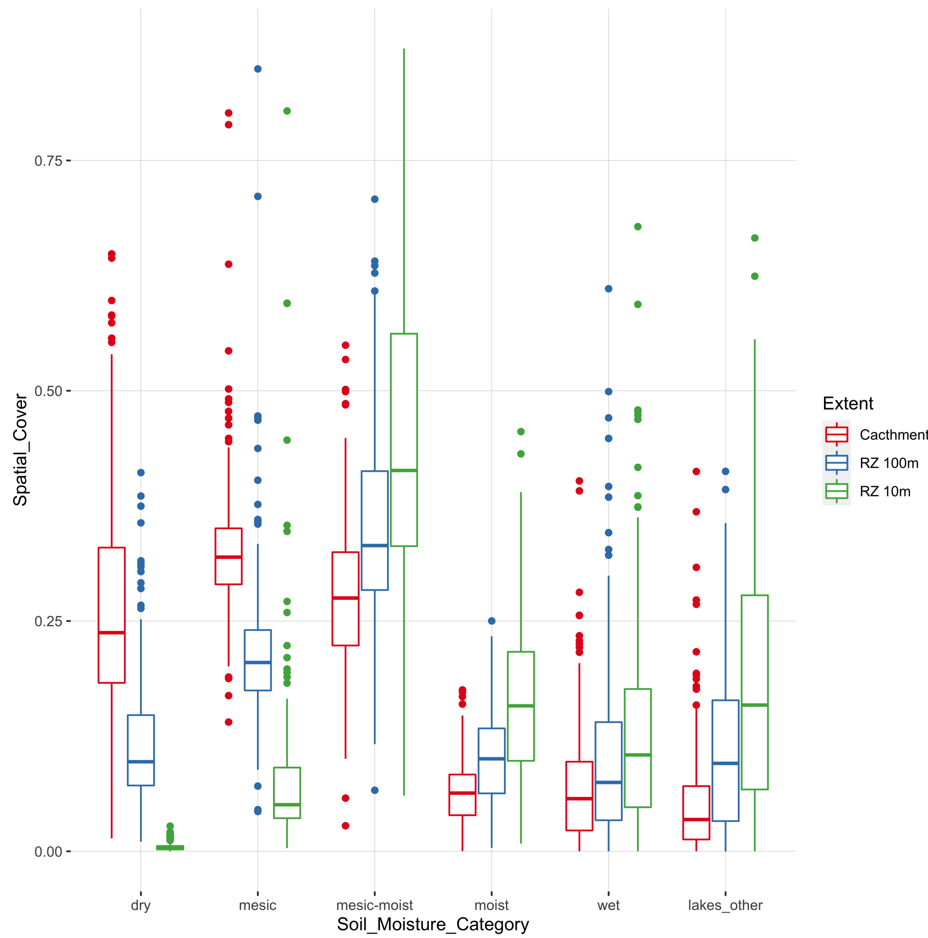

Fig. 6: Soil Moisture Cover for area within the RZ of 10 m FDS, and 100m FDS for a modeled stream initiation size of 10ha and for the entire catchment.

3.3 Principal Component Analysis

In using three principal components PCA was able to explain a total of 68.6% variation of high resolution derived variables without consideration to TOC data. The first principal component explained 44.5% of the variation in high resolution data, the second principal component explained 15.4%, and the third principal component explained 8.7%. The loading plot for the first two principal components is shown in Figure 7. A cluster analysis of the PCA loadings for all principal components using five clusters grouped the variables together largely corresponding to the soil moisture type. Changes in SMC with changing stream initiation size, SMC near stream, and SMC of the entire catchment all grouped together for each SMC type. Wet and moist SMC grouped into one cluster together. The cluster termed 'other' includes stream length changes and stream density as well as two SMC variables, dry SMC within 10 m of the stream for a stream initiation size of 30ha and the change in dry SMC from 30ha to 10ha within 10 m of the stream.

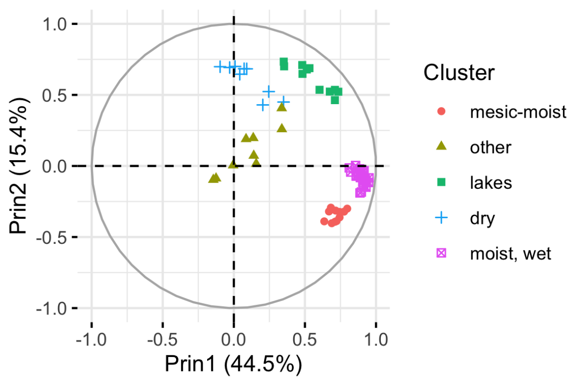

Fig. 7: PCA loading plots for the first two principal components explaining a total of 59.9% of the variation in variables. The 62 variables used were split into 5 clusters by k-mean clustering. The clusters contain the SMC of the soil type specified, except for the others cluster which includes area, elevation, stream length changes and stream density, as well as dry SMC for a 30ha stream initiation size and the change in dry SMC from 30ha to 10ha stream initiation size.

3.4 Projection to Latent Structure Regression

3.4.1 TOC influences

PLS regression using TOC and influences of the parameter parsimonious model were able to be fit models with explanatory power using high resolution and traditional data with Q^2 above 0.90 for all combination of x-variables (Table 4). The combination of high resolution and traditional variables was able to explain the most variation in the response variables while also having the highest Q^2. Using only high resolution was able to explain 40% of the variation in response variable, while traditional data and the combination of both was able to explain 64, and 65% respectively. Of the explained variation for all PLS models TOC had a higher variation explained than the discharge, trend and seasonality influences, see Figure 8. The greatest reduction of response variability explained when comparing a PLS with all x-variables and only using high resolution data as x-variables occurs for the Flow Coefficient.

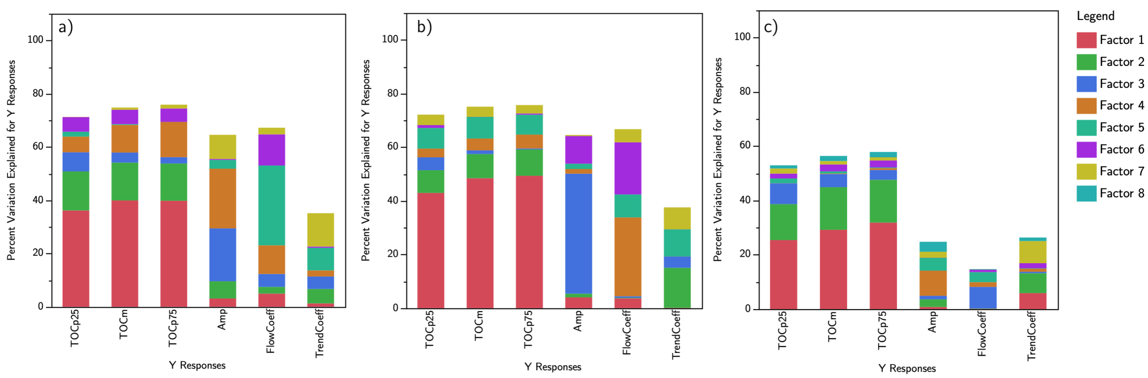

Fig. 8: Variation of TOC ($TOC_{P25\ \&\ P75}$,TOC_m) seasonality influence (Amp), flow influence (FlowCoeff), and trend influence (TrendCoeff) on TOC explained by (a) traditional data, (b) traditional and high resolution data, and (c) only high resolution data as found by PLS models for the corresponding variables. The variation explained is further split into the principal components (factors) of the PLS model used.

For the PLS model using all available data the variables with the greatest VIP score (VIP > 1.3) are by order of descending importance: Sand Sorted % (2.25), Coniferous Forest in Wetlands % (1.84), Elevation (1.65), C:N $Soil_{sd}$ (1.58), Specific Discharge[2] (1.0-1.6), Peat % (1.55), Pine Biomass (1.50), Lakes % (1.44), Discharge[3] (1.30-1.42), T_{max} (1.41), Rösberg (fractured bedrock) % (1.39), area (1.35). The highest coefficients showed TOC has a positive relation to Coniferous Forests in Wetlands, peat, temperature and pine biomass while it has negative relation to the sorted sand fraction, elevation and specific discharge. For the seasonality, the amplitude was positively influenced by water % and negatively related to the sorted sand fraction, coniferous forests in land use and specific discharge. The flow coefficient was most influenced negatively by the the variation in discharge and positively influenced by the sorted sand fraction. The trend coefficient was most influenced by the silt-sand fraction positively and negatively by peat %. For a complete list of VIP scores and corresponding coefficients for the PLS using all data see Supplementary Table S1.

[2]Includes basic statistics for Specific Discharge: mean (1.68), max, min, and standard deviation, 25^{th} percentile, 75^{th} percentile

[3]Includes basic statistics for Discharge: mean (1.42), median, max, min, and standard deviation, 25^{th} percentile, 75^{th} percentile

Table 4: Table of R^2, the amount of variation of the response variables the model can explain, and Q^2, the efficiency of the model, for PLS models calculated. Two different set of variables were predicted: long term trend analysis results (TA) from Eklöf et al. (2021) and parameter parsimonious model (PPM) results from Hytteborn et al. (2015). Additional mean TOC, the 25^{th} and 75^{th} percentile of TOC were predicted in each model. Three sets of predicting variables were used, traditional data, high resolution data, and all data: the combination of both.

		Q^2	R^2	Factors	VIP	Catchments
PPM	Traditional Data	0.93	0.64	6	25	133
	High resolution Data	0.90	0.40	8	87	134
	All Data	0.97	0.65	7	106	133
LTA	Traditional Data	-0.04	/	/	/	154
	High Resolution Data	-0.07	/	/	/	151
	All Data	-0.04	/	/	/	149

For the PLS model using only high resolution data 30 of 32 variables had a VIP score greater than 0.8 and 13 greater than 1.0. Figure 9 shows the importance, magnitude and direction of influence on each response variable by each predictive variable. Elevation had the highest VIP score with a positive influence on amplitude and the flow coefficient and a negative influence on TOC and the trend coefficient. The amplitude was most influenced by stream contraction and lakes in catchment, both having a negative influence and a greater magnitude than elevation and area. For TOC, the flow coefficient and the trend coefficient elevation and area had the greatest influence.

3.4.2 Long term TOC trend

No model with explanatory power was able to be fit to explain variation in the TOC and time fraction data from Eklöf et al. (2021), using high and/or traditional data as a 10 fold validation found a Q^2 of -0.04, -0.07, and -0.04 (Table 4).

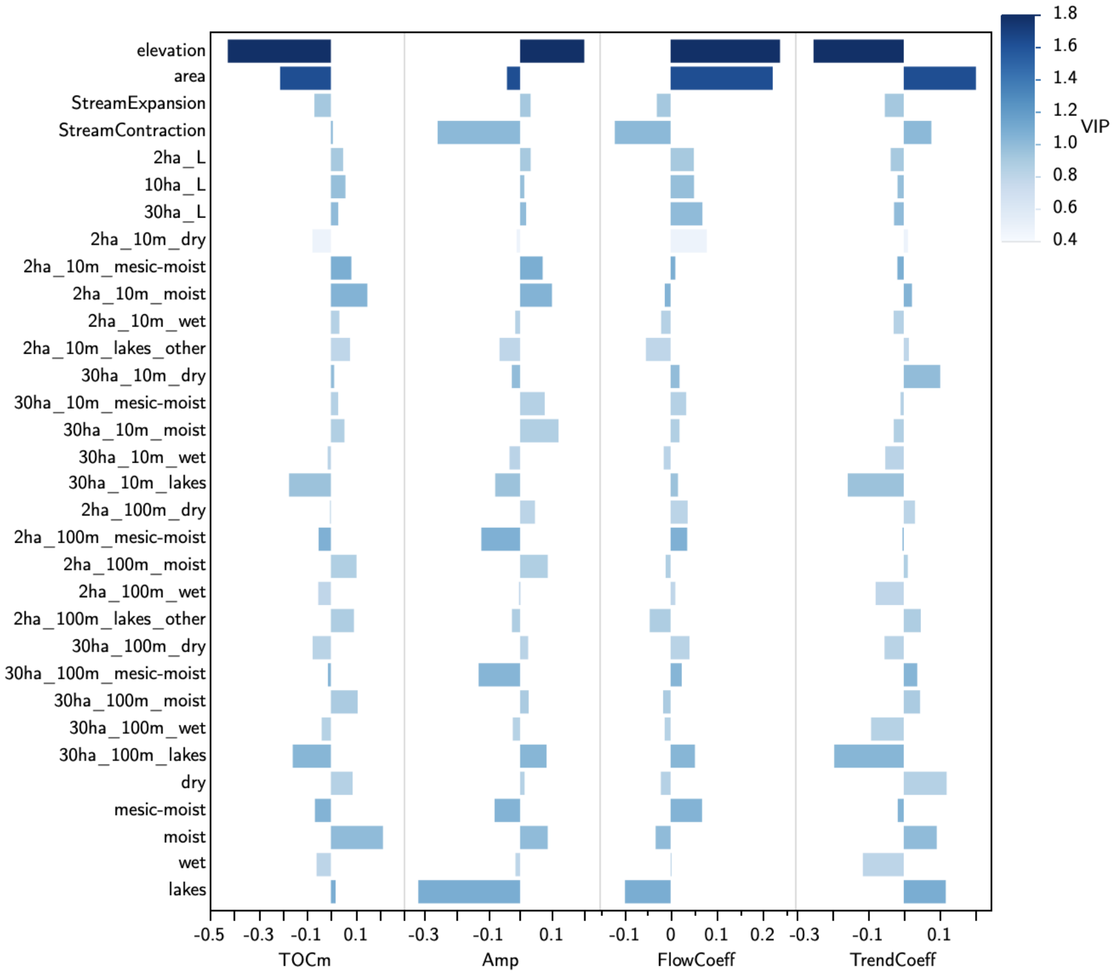

Fig. 9: Coefficients for the variables of the PLS using High Resolution data to explain variation in TOC and the influence of seasonality (Amp), flow (FlowCoeff), and trend (TrendCoeff) on TOC variability. For variables of the form xha ym the SMC of the area added to the area y meters near stream when considering a change from x ha stream initiation size to 10 ha stream initiation size. Variables labeled with only a soil moisture type represent the coverage of the entire catchment. Stream Expansion and Contraction are variables of the change in length of the river system changing from a 10ha stream initiation size. L is the stream density.

4 Discussion

4.1 Riparian Zone

In the boreal region low lying RZs with high OM content are commonly found in the headwaters. Assuming moister soils to have greater mobile OM concentrations, this is supported by the mean SMC shifting towards drier soil moisture categories the more area further away from the stream is considered. As topographic indexes such as Depth to Water were used in the creation of the SMM, moister areas accumulate closer to stream. Mineral soils found further away from the stream are generally drier and as such the SMC of the entire catchment shifts towards drier SMC categories , such as dry and mesic (Figure 6). For catchments typical of the Swedish region the RZ is defined as the zone between streams and the transition to these dryer mineral soils, associated also with a shift in vegetation from mosses and norway spruce to vaccinium shrubs and scotts pine (Ledesma et al. 2018). Within forestry a fixed buffer is commonly used to determine RZ protection measures. Considering the RZ as a fixed distance, though functionally practical, has been argued to miss the spatial variation of the RZ and therefore to adequately protect the RZ (Laudon et al. 2016). Ledesma et al. (2015) found the RZ to vary in width between 2 and 93m. Though the importance of RZ width has been supported by studies at catchment scale such as Ledesma et al. (2015) and Grabs et al. (2012) upscaling these findings to cover larger areas remains a challenge. RZ width is commonly determined using field observations of vegetation, terrain, and soil type, limiting the ability of RZ width to be determined for large scale analysis. High resolution digital mapping presents an alternative way of characterizing the RZ which can be done at a large scale, as it can minimize manual labor and cover large areas at a time. High variability of RZ width suggests the need for a high resolution. Considering a variation in RZ of 2-93m using traditional soil type data with an effective resolution of minimum 25m may miss important detail compared to high resolution data of 2m. Using the SMM to characterize near stream SMC may present a method for characterizing RZ width at a large scale. Characterizing the SMC within 100m may able to serve as a proxy for determining RZ width with areas where the SMC is drier RZ width is shorter.

The clusters for the PCA loadings of the high resolution variables clustered naturally according to their soil moisture category with the exception of the dry SMC within 10m of the stream (Figure 7). This suggests that although the SMC changes when including more area further from the stream, as a significant difference in all SMC of all soil moisture categories between 10m and 100m was found, the variation of these changes between catchments follow similar trends. 68% of variation within 62 variables can be captured by 3 principal components suggesting that a majority of the variation are dependent on similar underlying factors which are captured by the characterisation of the whole catchment. Since the PCA is an unsupervised form of dimensions reduction, the variation which is excluded when generalizing the variables according to the soil moisture type may contain important information. Though contrary to the expectation there lies no clear evidence in the VIP scores of the PLS results indicating that variables extracted near the stream are of greater importance than the SMC of the entire catchment (Figure 9). This suggests that the RZ reflects the spatial composition of soil moisture of the catchment and supports a generalization approach of soil moisture for the entire catchment.

4.2 Spatial component of parameter parsimonious model of TOC

The change in variation explained for TOC and TOC influences, by adding high resolution data to traditional data is minimal as only traditional data explains 64%, and both together are able to explain 65%. Both flow (Erlandsson et al. 2008) and temperature (Winterdahl et al. 2014) are known to be significant predictors of DOC concentrations, neither of which were included in the high resolution PLS model, leading to the decrease in explained variation between all data PLS and high resolution data PLS. Though the high resolution data does not provide additional explanatory power on its own high resolution can explain 40% of the variation, suggesting it does not add new information but it contains relevant information of importance. Looking closer at how which variables contribute to the explanatory power of the high resolution only PLS model, may therefore tell us about the characteristics of the catchment influencing TOC concentrations. For all three PLS models the variables were able to explain mean TOC, TOC_{P25}, and TOC_{P75}, to a greater extent than the three influences of discharge, seasonality, and trend (Figure 8). Additionally, the variation explained for the influences decreased more drastically for the influences when excluding traditional spatial data than for mean TOC. Both of these suggest that both topographic variables such as the high resolution data as well as other spatial characteristics contained in the traditional data are able to quantify the mean TOC but are less suited for investigating the behaviour of TOC concentration as characterized by TOC influences of seasonality, flow and trend in more detail.

In looking at the variables of greatest importance to each PLS model, processes determining TOC and its variation can be identified. First processes identified by the traditional data are identified, to then relate these processes to the explanatory power of the high resolution data and their variables of importance. For mean TOC the most important variables when using traditional data are related to climate (maximum temperature and elevation) and spatial variables related to biomass accumulation and decomposition:

Table 5: Summary table of the most important variables for TOC and TOC influences, including the direction of the linear relation. For each TOC influence and mean TOC the key process as highlighted by the important variables is included in the box below the variables.

	TOC		Seasonality		Flow		Trend	
Traditional Data	ConiFor Wet% +	Carbon Pool Size	Lakes% -	Buffering	Sand Sorted% +	Flushing	Peat% –	Compilation
	Peat% +		Water% -		Silt sand unsorted% +		Q_{cv50} +	
	Elevation –		Sand Sorted% +		Tot Sand% +		Q_{scv50} +	
	T_{max} +		Lag Time –		Tot silt sand% +		Wetland% -	
	DeciFor Wet% +		Residence Time –		CleFel For% +		OpenWet% -	
	MixFor Wet% +		ConiFor Wet% +		BirchM -		Sand Sort% -	
High Resolution Data	Elevation -		Lakes -		Elevation +		Elevation –	
	Moist +		Stream contraction -		Area +		Area +	
	Area -		Elevation +		Stream Contraction –		30ha,100m lakes -	
	30ha,10m lakes -		30ha,100m mesic-moist –		Lakes –		30ha,10m lakes –	
	30ha,100m lakes -		2ha,100m mesic moist –		2ha,10m dry +		Dry +	
	2ha,10m moist +		30ha,10m moist +		30ha L +		Lakes +	

coniferous forested, deciduous forested, and mixed forested wetlands, and peat (Table 5). Though these variables interact with all three determinants of TOC: carbon pool size, mobility, and transport; they emphasize the control of the available carbon pool through the spatial extent of accumulation and slow decomposition of biomass wetlands and peat soils are associated with due to their high water table. The spatial variation of the impact of seasonality on TOC variation is negatively related to the amount of lakes and open water, and the time aspect of the movement of water through the catchment (lag time, residence time) (Table 5). This suggests that the influence of seasonality is controlled by buffering processes, processes which dampen variation. As lakes function as buffers reducing TOC variability, the more lakes are included the less influential the seasonality becomes. Additionally, the longer water spends time in the catchment the more the TOC variation can be buffered, hence also reducing seasonal variation.

The impact on flow on TOC variation is most influenced by coarser sediments of silt and sand (Table 5). In headwaters a narrow layer in the riparian profile is responsible for up to 90% of the DOC export (Ledesma et al. 2015). Hydraulic conductivity changes exponentially with depth (Nyberg 1995), so changes in the water table lead to changes in the dominant flow path and may shift the dominant source layer for DOM. Soils with more coarse sediment have a greater fluctuation of their water table as the hydraulic connectivity along the profile have a less distinct exponential decrease compared to soil profiles with more fine sediment. Additionally soil layers which are not continuously hydrologically connected to stream may accumulate OM that can be flushed out of the soil and into the stream when intermittently connected to the stream. Flushing refers to the build up of a solute which is then exported during events of high flow or increased hydraulic conductivity (Burns 2005). Flushing can occur with changes in the lateral connectivity of the catchment as well as the vertical component of the lateral flow and the shifting of the dominant source layer of organic matter vertically along the soil profile. The high importance of coarse sediment for the impact of flow on TOC variation therefore suggests flushing as a dominant process. As a greater variation in hydraulic connectivity both horizontally and vertically associated with the hydraulic connectivity of coarser sediment increases the dependents of TOC variation on flow.

The variables of most importance for the trend influence on TOC variation are less clearly pointing at one specific dominant process but instead point at a combination of carbon pool size (wetland%, and open wetlands%, peat%) and the hydrologic regime and transport of water through the catchment (discharge and specific discharge coefficient of variation, sand sorted%) (Figure 5). However, the model was only able to explain the trend coefficient with less than 40% explanatory power, the least explanatory power of all predicted variables (Figure 8). The interplay of various determinants and processes of TOC variation that are important for the trend influence and the low explanatory power of the PLS model for the trend coefficient suggest that the influence of trend more so than the other explained variables is unable to be explained using traditional and high resolution catchment characteristics. Consequently the importance of processes and characteristics that have been excluded from this analysis is highlighted.

The potential explanatory power of the SMM for TOC variation is based on the key assumption that OM accumulates in areas with high soil moisture. High resolution data from the SMM is able to best explain mean TOC (Figure 8), the predicted variable connected most closely to the carbon pool size of the catchment when looking at the PLS which uses traditional data. Based on the assumption and supported by the results high resolution data is therefore able to better capture the carbon pool size, while it is not able to capture the processes and variables important for TOC influences as well. Buffering and flushing are both less represented in the data the SMM can provide. In terms of buffering lakes are included in the high resolution data but no consideration is given to other components of the hydrological regime of the catchment and the resulting time water and DOC spends in the catchment. The importance of flushing may, however, be reflected in the higher VIP of mesic-moist soils. VIP scores for variable coefficients show that mesic-moist soils are generally more important than wet soils (Figure 9). The importance of mesic-moist soils, especially for positive relation to the flow coefficient, may be explained by flushing. While wet soils are more likely to be connected to the stream system for extended periods, mesic-moist soils may accumulate DOM and during periods of high flow become intermittently hydrologically connected to the stream system through a shift in the vertical and horizontal hydraulic connectivity. A three dimensional view of the catchment emphasises the role of flushing in the export of OM from upslope areas (McGlynn and McDonnell 2003). Mesic-moist soils are therefore not only important in the RZ but also in the entire catchment as supported by similarly high VIP scores for mesic moist soils within 100m as within the entire catchment.

Variables used for the analysis capture horizontal variability in carbon pool and some aspects of horizontal hydraulic connectivity through the use of the SMM and changes in the extent of the stream system. However, TOC behaviour may depend not only on the horizontal variation of the carbon but also on the vertical variation in carbon pool and transport. This vertical component to the export of DOM may be one of the reasons the horizontal variability captured in the high resolution data is unable to predict TOC influences for more than 20%.

4.3 Spatial component of long term TOC trend analysis

Neither traditional data nor high-resolution data was able to fit a model with predictive power for explaining changes in long-term trend changes as found by Eklöf et al. (2021). This suggests that the mechanism determining the change in trend were not captured by either data set. Both the traditional data and the high resolution data used as explanatory variables are stationary in time and do not represent temporal changes. However, long term trend changes are found as a function of time. This lack of representation of temporal variation may explain the lack of explanatory ability of the variables used. For example changes in biomass and associated changes in the available soil carbon pool are not captures within the variables used but may be driving DOC trend changes. In southern Sweden agricultural land was converted to forest in the early 1900s (Lindbladh et al. 2014). This caused an increase in forest biomass which is suggested to be driving brownification in southern Sweden (Kritzberg 2017; Škerlep et al. 2020). In addition forests in southern Sweden have shifted form being dominated by *Pinus* (pine) to *Pinea* (spruce) (Lindbladh et al. 2014). In Sweden spruce dominated forest stands have been found to have greater soil organic carbon stocks and soil organic carbon accumulation than pine forest stands (Stendahl et al. 2010). Changes in land use from agriculture to forestry and spruce dominated forest stands may therefore explain continued brownification in southern Sweden through an increase in carbon pool size. Southern Sweden also experienced greater acid deposition and may therefore be taking longer to recover from acidification resulting in continued brownification (Eklöf et al. 2021). Continued brownification is also occurring in the northeast of Sweden, an area experiencing isostatic rebound since the last glaciation period leading to paludification and the accumulation of OM of the new emerging land (Tuittila et al. 2013).

DOC variation and trend are influenced by changes in the size, mobility and transport of the carbon pool. All three of these determinants may be influenced by temporal changes in land use/ land cover, changes in precipitation and temperature as well. The high resolution data extracted from modeled stream networks and SMM is not be able to capture data on change, and therefore unable to explain the changes in long term trends found by Eklöf et al. (2021). For future spatial analysis that aims to explain the spatial variation of DOC trend changes, it is therefore seen as necessary to include data on change within a catchment as well as temporally stationary catchment characteristics. This may include temperature changes, precipitation changes, as well as land use and biomass/ vegetation changes.

4.4 Limitations and Outlook

The use of digital maps can provide a way to characterize the catchment based on continuous spatial information, however, there are a few limitations that come with the current state of digital maps. One of the main limitations of this analysis is the inconsistencies in the spatial data used. For example the vector files delineating the catchments where not consistent in placing the watershed boundaries, causing overlaps and complicating the analysis (see Figure S1). Not only did catchment boundaries overlap but they did not align perfectly with the stream system causing some streams to be excluded from the catchment even though they are upstream of the monitoring station. Visible inspection showed there was little consistency to the direction and magnitude of the inconsistencies. This inconsistency is assumed to come from the different systems used to create the catchment boundaries: catchment boundaries for the 215 catchments with monitoring stations at the outlet were digitized using the hydrological network VIVAN which is based on a 50m DEM (Nisell et al. 2007); the 2 818 sub catchments were delineated directly using whitebox tools based on a DEM of 50m resolution.

When calculating stream lengths, the stream systems had to exclude areas of open water as these are mapped as randomly crossing streams in the open-source modeled stream networks. In the case of this thesis this was done by using the open waters of the Swedish properties. Similar to the catchment boundaries the accuracy of the calculations were limited by the inconsistencies between the maps used. The open water from the property map was able to remove most random streams that occur where there is open water but not all. Additionally the open water map removed any streams which can be found in the open water map. Therefore, the calculation of stream length is not a calculation of the entire stream network of a catchment, but instead a calculation of the stream network not shown on the Swedish property map. For this reason caution is given to the use of absolute numbers calculated in stream length and SMC. Instead the focus in the multi-variant analysis was given to changes, to eliminate some of misinformation that occured as a result of extra streams and missing streams. Within the use of high resolution geospatial data there is a trade-off between capturing the most detailed accurate information and processing power or time. For the purpose of this thesis the need to minimize the processing power needed was prioritized leading to sources of inaccuracies that if sufficient time and processing power was available may be avoided. Delineation issues for example could have been minimized by re-digitizing all catchment boundaries using the same methods. Digital maps are increasingly published as open data sources which makes projects such this thesis possible. However, limitations such as inconsistencies discussed above need to be considered when working with digital maps based on different sources.

High resolution modeled stream systems are able to more accurately capture the stream network of catchments than traditional topographic maps (Lidberg et al. 2017); while the temporal dynamics of a stream network can be represented by using different stream initiation sizes (Ågren et al. 2014). Similar to traditional maps missing small streams, both traditional maps and high resolution modeled stream networks miss mapping artificial ditches. Hasselquist et al. (2018) found in a small catchment in norther Sweden ditches nearly doubled the length of the stream network. In Sweden most ditches were dug before modern mapping techniques, and therefore there is no account of where and how many artificial ditches there are (Hasselquist et al. 2018). Ditches change the hydrology of the catchment by altering the quantity, quality, and dynamics of water moving through the catchment (Price et al. 2003). Artificial ditches were historically dug to increase the productivity of land by lowering the groundwater table and making conditions more favorable for root growth (Sikström and Hökkä 2016). Artificial ditches are mostly dug to drain peatlands though ditches have also been dug through well drained sedimentary soils (Hasselquist et al. 2018). Recent findings suggest that drainage of peatlands may not only have a short term impact on DOC concentrations (Joensuu et al. 2002) but also responsible for long term changes (Nieminen et al. 2021). Although developments of ditch data are ongoing and can be found on the Swedish forestry website similar to the modeled stream networks, all consideration of artificial ditches was excluded from this thesis. This is due to the vast amount of big data that the information on ditch networks includes, which exceeded the computational capacity of this thesis. However, in further developing the approach of using high resolution digital mapping to characterize the headwaters and explain variation in DOC trends and patterns the inclusion on ditch data is seen as an essential step.

5 Conclusions

Contrary to the expectation there is no clear evidence suggesting that the RZ is more important than the SMC for the entire catchment. Similarly, the hypothesis of increased flow influence for catchments with greater moist area added to the stream when changing from 10ha to 2ha stream initiation size, is not supported by the data. Although the results of this study were unable to support either of the hypothesis, this study showed the ability of high resolution soil moisture and stream length data to explain variation in DOC trends and patterns. High resolution data was able to explain 40% variation in TOC concentration, and TOC influences of flow, seasonality and trend. Traditional data with a minimum spatial resolution of 25m was able to explain 65% with no additional explanatory power if high resolution data was added. So overall, traditional data already encompasses a lot of information about the catchment that is able to partially explain some TOC variation and adding high resolution soil moisture data does not add new information. This may in part be because the SMM is based on the traditional data. It also suggests that the remaining explanatory power may lie in catchment characteristics and processes not considered by the included data such as vertical variability . In conclusion, the high resolution data did not capture any information of the underlying factors controlling TOC behaviour that was not already included in the traditional data. This emphasizes the importance of catchment characteristics that were not captured by any of the data such as changes in SOM, and the vertical distribution of the SOM, as well as changes in hydrology through drainage ditches. In addition to explaining spatial DOC variation this study was able to use the SMM to characterise the riparian zone across an extended area and various catchment sizes.

Management decisions are based on predictions and considering the importance of the carbon cycle on essential current management decisions concerning the climate crisis as well as local resource management, understanding and predicting components of the carbon cycle accurately is essential for management decisions on all scales from local to global. While the underlying mechanisms of TOC export have been studied, to a large extent it remains a challenge to upscale the knowledge for accurate predictions at a national or global scale as the interaction of soil carbon pool size, mobility and transport vary in time and space within the headwaters of the catchment. This thesis highlighted the potential and limitations in using digital mapping to bridge the gap of spatial characteristics of the headwaters and data collected at the outlet. By overcoming current limitations of the consistency of digital spatial data and computer power digital maps may be used in the future to include additional information important in TOC export that can improve predictions and lead to better management decisions.

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Supplementary Material

Table S1: Coefficients of PLS model using all available data as x-variables with TOC (mean and percentiles) and seasonal, trend, and discharge influences on TOC as found by Hytteborn et al. (2015) as y-variables.

Variable	TOCp25	TOCm	TOCp75	Amp	FlowCoeff	TrendCoeff	VIP
2ha_10m_dry	-0.03048	-0.02973	-0.02739	-0.01023	0.03778	0.003662	0.591321
2ha_10m_lakes_other	0.018617	0.005614	-0.0008	-0.04871	-0.04714	-0.01754	0.855862
2ha_10m_mesic-moist	0.028209	0.028299	0.028637	-7.6E-06	0.000199	-0.0268	1.211073
2ha_10m_moist	0.043196	0.043348	0.043116	0.007345	-0.01245	-0.02236	1.257487
2ha_10m_wet	0.018639	0.019099	0.019751	0.003249	-0.00212	-0.0218	0.866003
2ha_100m_dry	-0.00778	-0.00586	-0.0041	0.000644	0.020291	0.02979	0.556061
2ha_100m_lakes_other	0.006975	-0.00352	-0.00867	-0.04204	-0.03318	-0.00724	0.714299
2ha_100m_mesic-moist	0.02878	0.026003	0.02505	-0.01305	-0.0012	-0.02098	1.090747
2ha_100m_moist	0.031342	0.032088	0.032435	0.009861	-0.0108	-0.00905	0.992233
2ha_100m_wet	0.004946	0.006061	0.007457	0.004835	0.004678	-0.01428	0.698187
2ha_L	0.010181	0.020815	0.026394	0.030216	0.060607	-0.00676	0.990395
10ha_L	0.016576	0.026182	0.031067	0.026915	0.056351	-0.00328	1.043173
30_10m_wet	0.003894	0.00571	0.007425	0.004985	0.008834	-0.02399	0.744535
30ha_10m_dry	-0.01766	-0.01839	-0.01839	-0.00274	0.002521	-0.0094	0.775996
30ha_10m_lakes_other	-0.01501	-0.02435	-0.02775	-0.04109	-0.01834	-0.0307	0.92167
30ha_10m_mesic-moist	0.009606	0.012351	0.01437	0.007504	0.01394	-0.02359	0.843131
30ha_10m_moist	0.012629	0.01611	0.018464	0.013639	0.012465	-0.02495	0.910525
30ha_100m_lakes_other	-0.022	-0.02935	-0.03187	-0.03277	-0.01069	-0.02686	0.868661
30ha_100m_mesic-moist	0.025155	0.024065	0.024086	-0.00929	0.006956	-0.01488	1.049539
30ha_100m_moist	0.029157	0.030949	0.032037	0.009412	0.001732	-0.01418	1.021188
30ha_100m_wet	0.007084	0.008103	0.009221	0.004821	0.001283	-0.02353	0.728411
30ha_L	0.018188	0.026849	0.031251	0.024536	0.051687	0.00016	1.039574
30ha_pt_100m_dry	-0.00212	-0.00095	0.00024	-0.00035	0.013752	0.018393	0.451992
AgeM	-0.03959	-0.03407	-0.03072	0.016623	0.027872	-0.0022	1.162758
Agri%	-0.01435	-0.0179	-0.01962	-0.01505	0.000318	-0.00633	0.642296
area	-0.01497	-0.01875	-0.0204	-0.00908	0.002753	0.025656	1.353258

Variable	TOCp25	TOCm	TOCp75	Amp	FlowCoeff	TrendCoeff	VIP
Bedrock%	-0.0028	-0.01375	-0.01946	-0.03623	-0.06496	0.029278	0.992302
BeechM	-0.0302	-0.03192	-0.03253	-0.0016	-0.00287	-0.00443	0.830087
BiomM	0.037389	0.034953	0.032626	-0.00052	-0.03302	0.030713	1.144988
BirchM	0.029411	0.018238	0.011407	-0.0298	-0.06224	0.016617	0.851404
Block%	-0.04559	-0.03971	-0.035	0.012435	0.051241	-0.00328	0.824104
C_dry	-0.01065	-0.00739	-0.00523	0.005003	0.018169	0.037769	0.623371
C_lakes	-0.00041	-0.01655	-0.02405	-0.06738	-0.04568	0.003104	1.097656
C_mesic_moist	0.02593	0.025228	0.025446	-0.00776	0.013799	-0.02061	1.097562
C_moist	0.037152	0.040975	0.042732	0.01763	0.00709	-0.01043	1.131755
C_wet	0.009582	0.010719	0.011665	0.006667	0.000793	-0.02521	0.695114
Clay%	-0.01266	-0.01972	-0.0223	-0.03075	-0.01603	0.013129	0.542699
ClayBlock%	-0.02	-0.02711	-0.02976	-0.02954	-0.01372	0.004138	0.62623
ClayBlockSort%	-0.03055	-0.02108	-0.01518	0.035641	0.065135	-0.02348	0.971679
ClayBlockUnsort%	-0.01337	-0.01106	-0.00958	0.006623	0.004674	-0.01215	0.621008
ClaySandUnsort%	-0.01145	-0.01684	-0.0201	-0.01685	-0.02509	-0.01369	0.756643
ClaySilt%	0.000882	-0.00562	-0.00919	-0.02276	-0.03687	-0.00204	0.504216
ClaySiltSort%	-0.01871	-0.0283	-0.03262	-0.03755	-0.02431	-7.5E-05	0.813084
ClaySiltUnsort%	-0.00677	-0.0118	-0.01403	-0.01913	-0.01393	0.002274	0.355847
ClaySort%	0.011166	0.003097	-0.00102	-0.03562	-0.02592	0.028344	0.734011
ClayUnsor%	0.024517	0.018857	0.013857	-0.01271	-0.05069	-0.01863	0.754546
CleFellFor%	-0.0147	-0.00879	-0.00363	-0.00415	0.07598	0.018722	1.098798
CNsoilM	-0.03803	-0.03727	-0.03579	-0.00566	0.015872	-0.00687	1.170792
CNsoilSd	-0.04345	-0.0378	-0.03426	0.02501	0.036756	-0.00561	1.584019
ComArea%	-0.02634	-0.0257	-0.02423	-0.00748	0.037499	-0.00755	0.651915
ConiFor%	0.009197	0.011553	0.013132	0.001672	-0.00135	0.035351	0.911524
ConiForWet%	0.07014	0.081219	0.084575	0.063543	-0.00048	-0.01419	1.848061
ContortaM	-0.03217	-0.04204	-0.04513	-0.04946	-0.01501	0.022561	0.988734
CorrLag	0.031153	0.03008	0.027733	0.010452	-0.03181	0.005488	0.710726
CropAgri%	-0.01584	-0.02002	-0.02213	-0.0173	-0.00458	-0.00858	0.68506
CsoilM	0.039437	0.043015	0.043397	0.027236	-0.00129	-0.01839	1.154793

Variable	TOCp25	TOCm	TOCp75	Amp	FlowCoeff	TrendCoeff	VIP
CsoilSd	-0.00396	-0.00617	-0.00736	-0.0076	0.005297	-0.03145	0.680219
DeciFor%	-0.04005	-0.03504	-0.03164	0.025843	0.027402	-0.02511	0.966643
DeciForWet%	0.050155	0.046867	0.044148	-0.01596	-0.01236	-0.01349	1.093992
DeciM	0.010707	0.007474	0.00484	-0.00365	-0.02265	-0.00165	0.517443
elevation	-0.07371	-0.06622	-0.06018	0.018714	0.063166	-0.02075	1.656971
Filling%	-0.01824	-0.01544	-0.01278	-0.00238	0.049402	-0.001	0.638638
For%	0.012984	0.020814	0.025304	0.024607	0.023261	0.024129	1.15049
ForNoWet%	-0.00321	0.000729	0.003336	0.011731	0.00193	0.02668	0.801015
GravelSort%	0.007598	0.005325	0.004535	-0.01729	0.002057	0.019747	0.529939
GravelUnsort%	-0.02853	-0.03133	-0.03129	-0.01344	0.003156	0.022913	0.617798
Gravitationsjord%	0.016649	0.025111	0.027704	0.048316	0.010836	0.012228	1.131836
HeigM	0.021851	0.026737	0.028483	0.025172	0.004742	0.021471	0.987924
Ice%	0.015429	0.0235	0.025889	0.04753	0.008988	0.010461	1.148748
LagTime	0.008442	-0.00677	-0.0137	-0.06695	-0.03889	0.032512	1.094718
Lake%	-0.01923	-0.03847	-0.04695	-0.07993	-0.0487	0.007873	1.441761
Lat	-0.00788	-0.01243	-0.01462	-0.02614	-0.01778	-0.01037	0.912008
Lime%	0.039069	0.035816	0.031893	-0.00495	-0.0428	-0.01176	0.703712
Long	0.030338	0.025878	0.022443	-0.02259	-0.02729	0.005252	0.861071
MixFor%	0.051355	0.042684	0.036581	-0.02698	-0.06725	0.007075	1.019165
MixForWet%	0.045618	0.046661	0.045836	0.006739	-0.01713	0.000637	0.925113
Mud%	0.050547	0.041568	0.035748	-0.03658	-0.0455	0.036375	1.205527
NsoilM	0.034191	0.036912	0.036925	0.022861	-0.00299	-0.0115	1.021241
NsoilSd	-0.00267	-0.00304	-0.00352	0.001733	0.010439	-0.01732	0.551095
OakM	-0.02888	-0.02702	-0.02586	0.018138	0.005258	-0.00666	0.842494
OpenWet%	-0.01195	-0.01574	-0.01737	-0.00968	-0.02349	-0.02943	0.821651
OthCultAgri%	-0.05781	-0.05231	-0.04664	0.002348	0.081961	0.039929	1.17748
OthDenseVegArea%	0.027177	0.027416	0.025295	0.014754	-0.02808	-0.03024	0.985123
OthPorVegArea%	0.019704	0.021365	0.020727	0.017588	-0.01677	0.017039	0.728012
OutSwe%	-0.01552	-0.01336	-0.01159	0.004698	0.030469	0.011306	0.594042
Pannual	-0.01537	-0.0142	-0.0134	0.03262	-0.03265	0.001853	1.187213

Variable	TOCp25	TOCm	TOCp75	Amp	FlowCoeff	TrendCoeff	VIP
PasAgri%	-0.00125	-0.00047	0.000252	0.001348	0.023488	0.006541	0.594384
Pcv	0.023309	0.016003	0.011862	-0.04859	-0.00284	0.006187	1.137083
Peat%	0.079375	0.080934	0.078868	0.025697	-0.0442	-0.03733	1.550617
PineM	0.055946	0.061064	0.062459	0.007204	0.013964	0.019564	1.499594
Pm	-0.01537	-0.0142	-0.0134	0.03262	-0.03265	0.001853	1.187213
Pmax	-0.00476	-0.00011	0.002625	0.013397	0.034148	-0.02528	0.567682
Pmed	-0.02784	-0.01936	-0.01476	0.051801	0.001977	-0.02698	1.183602
Pp25	0	0	0	0	0	0	0
Pp75	-0.01851	-0.01416	-0.01161	0.042487	-0.01394	-0.001	1.193581
Psd	-0.00943	-0.01192	-0.01313	0.018464	-0.04818	0.004344	1.112979
Qcv	0.007508	0.006572	0.005149	-0.00095	-0.04668	0.006601	0.890317
Qcv50	0.019145	0.019619	0.018124	0.012669	-0.05421	0.024686	1.065551
Qiqr	-0.02236	-0.02309	-0.02291	0.000367	0.018446	0.031823	1.347184
Qm	-0.00982	-0.0106	-0.0111	0.005447	0.009169	0.026201	1.396725
Qmax	-0.02011	-0.02191	-0.02242	-0.00198	0.012882	0.026611	1.42255
Qmed	-0.0052	-0.00627	-0.00713	0.005761	0.004072	0.023467	1.345957
Qmin	0.007136	0.011091	0.011966	0.029613	0.009744	0.018257	1.334593
Qp25	-0.00174	-0.00226	-0.00301	0.008651	0.003726	0.021512	1.315721
Qp75	-0.01146	-0.01211	-0.01247	0.005384	0.010828	0.027771	1.405541
QsCV	0.007508	0.006572	0.005149	-0.00095	-0.04668	0.006601	0.890317
QsCV50	0.019145	0.019619	0.018124	0.012669	-0.05421	0.024686	1.065551
Qsd	-0.02444	-0.02574	-0.02573	-0.00269	0.019067	0.03021	1.386678
QsIQR	-0.03749	-0.03519	-0.03331	0.034747	-0.02323	0.006679	1.330421
QsM	-0.06533	-0.05885	-0.05388	0.04739	0.015599	-0.00135	1.678794
QsMax	-0.03893	-0.0336	-0.03059	0.034602	-0.016	-0.00918	1.185567
QsMed	-0.04493	-0.04287	-0.04016	0.021459	0.030127	0.001549	1.327099
QsMin	-0.02206	-0.00852	-0.00135	0.062605	0.066836	-0.00222	1.389336
QsP25	-0.03719	-0.03159	-0.02731	0.026282	0.057514	-0.00093	1.353389
QsP75	-0.0504	-0.04561	-0.04184	0.042524	0.00997	0.005112	1.450338
QsSd	-0.02273	-0.02042	-0.01906	0.015703	-0.00921	-0.00356	0.646093

Variable	TOCp25	TOCm	TOCp75	Amp	FlowCoeff	TrendCoeff	VIP
RecArea%	-0.02922	-0.0322	-0.03222	-0.02226	0.026336	0.013776	0.712768
ResiTime	-0.02669	-0.03695	-0.04087	-0.05009	-0.01118	-0.00852	1.01612
Rösberg%	-0.02298	-0.01315	-0.00839	0.046467	0.039021	0.011431	1.391111
Sand-gravel_sorted%	0.004143	0.002389	0.001346	-0.00578	-0.00936	-0.0128	0.24076
Sand%	-0.01842	-0.02394	-0.02622	-0.02125	-0.01251	-0.0015	0.571641
SandSort%	-0.09544	-0.0665	-0.04716	0.06796	0.227045	-0.02725	2.515003
Sandstone%	-0.00998	-0.01617	-0.019	-0.02358	-0.01601	0.002238	0.488665
SandUnsort%	0.034911	0.035709	0.035134	0.012648	-0.01001	0.0203	0.954712
Silt-sand_sorted%	-0.05353	-0.05197	-0.04809	-0.01493	0.071865	0.04934	1.20791
Silt-sand_unsorted%	-0.01474	-0.00054	0.006912	0.047719	0.074803	-0.03543	1.0532
Silt-sand%	-0.01228	-0.01532	-0.01706	-0.00876	-0.01347	-0.00954	0.559132
Silt%	0.007429	0.003519	0.001508	-0.01662	-0.01272	0.006045	0.2773
SiltSort%	-0.01661	-0.01885	-0.01885	-0.02105	0.022135	-0.00229	0.526154
SpruceM	0.030906	0.030573	0.02981	0.010802	-0.02597	0.022528	1.087894
Stone-block_sorted%	0.037903	0.036043	0.03391	-0.00161	-0.02689	0.006021	0.700052
Stone-block_unsorted%	-0.00197	-0.00508	-0.00645	-0.01246	-0.00601	-0.00178	0.24083
Stone-block%	-0.00903	-0.00735	-0.00587	0.004629	0.020904	0.026583	0.495158
StoneSort%	-0.00461	-0.01004	-0.01196	-0.02304	-0.00724	0.023167	0.461571
StreamContraction	-0.01131	-0.02032	-0.02461	-0.03362	-0.03582	-0.00263	0.85824
StreamExpansion	-0.02845	-0.03033	-0.03068	-0.0043	-0.01571	-0.01107	0.873092
Talus%	-0.02988	-0.02684	-0.02436	0.013938	0.0202	0.000873	0.581364
Tcv	-0.04168	-0.03503	-0.03006	0.013604	0.053573	-0.00194	0.738963
Tcv50	-0.04745	-0.04026	-0.03557	0.019868	0.0383	-0.02544	1.016421
Tiqr	-0.01717	-0.01931	-0.02004	-0.01715	-0.0062	-0.01249	0.908302
Tm	0.027735	0.027385	0.026417	0.009634	-0.00794	0.016422	0.929039
Tmax	0.073559	0.067895	0.062736	-0.0155	-0.03867	0.029475	1.413488
Tmed	0.021489	0.021869	0.021471	0.012111	-0.00276	0.013731	0.871995
Tmin	0.01361	0.015773	0.016518	0.015875	0.007182	0.008362	0.841154
TotClay%	0.024845	0.014823	0.008279	-0.0358	-0.05438	0.008492	0.820568
TotClayBlock	-0.01964	-0.01547	-0.01284	0.013526	0.017095	-0.017	0.683077

Variable	TOCp25	TOCm	TOCp75	Amp	FlowCoeff	TrendCoeff	VIP
TotClaySilt%	-0.0009	-0.00827	-0.01223	-0.02619	-0.03895	-0.00203	0.561282
TotGravel%	-0.00849	-0.01193	-0.01259	-0.02196	0.003434	0.029069	0.588933
TotSand%	-0.00809	0.004615	0.012108	0.039555	0.085152	0.007115	1.230478
TotSilt%	-0.00068	-0.00524	-0.00707	-0.02455	-0.00166	0.004471	0.388288
TotSiltSand%	-0.05261	-0.04517	-0.03886	0.009367	0.090308	0.019533	1.114538
TotStoneBlock%	0.03741	0.035184	0.032899	-0.00312	-0.02743	0.005801	0.68471
TotTill%	0.022751	0.023505	0.022405	0.01441	-0.02756	-0.00505	0.501129
TotVolM	0.037899	0.037219	0.035751	0.005951	-0.02514	0.026831	1.164205
Tp25	0.026556	0.026211	0.025315	0.009609	-0.00745	0.017075	0.928293
Tp75	0.032999	0.030589	0.028378	0.002754	-0.01851	0.020004	0.930034
Tsd	-0.02196	-0.02425	-0.02483	-0.01814	-0.00418	-0.01251	0.958109
Unknown%	0.004069	-0.00227	-0.00538	-0.02638	-0.02423	0.00454	0.437269
UrbArea%	-0.01358	-0.02096	-0.02432	-0.03135	-0.00869	-0.00791	0.710705
Volume	-0.005	-0.00782	-0.00966	-0.00028	-0.00949	0.01849	1.213198
Water%	-0.0135	-0.03265	-0.04128	-0.07873	-0.05014	0.007633	1.376703
Wet%	0.03226	0.035037	0.035355	0.025665	-0.02051	-0.03133	0.928323

Table S2: Variables used for analysis as traditional data and specific sources adapted from Hytteborn et al. (2015).

Type of data	Source map/model	Reference
Area and elevation	50m DEM	Swedish National Land Survey
Retention time	computed by Hytteborn et al. (2015)	Sobek (2011)
Discharge	S-HYPE at SMHI	Lindström et al. (2010) and Strömqvist et al. (2012)
Temperature and precipitation	PTHBV database with 4 km grid based on stations	Johansson (2002)
Land use	CORINE 2000	Bossard et al. (2000)
Soil type	Geological Survey of Sweden	SGU (2012)
Forest geographical data	kNN database from *Department of Forest Resources Management, SLU*	Reese et al. (2022)
Carbon and Nitrate in soil	modeled by Hytteborn et al. (2015)	

Table S3: Clusters of loadings found by PCA for 62 high resolution variables

		Clusters		
dry	mesic-moist	moist	lakes	other
dry	mesic-moist	moist	lakes	area
dry$_{\text{2ha, 10m}}$	mesic-moist$_{\text{2ha, 10m}}$	wet	lakes$_{\text{2ha, 10m}}$	elevation
dry$_{\text{2ha, 100m}}$	mesic-moist$_{\text{2ha, 100m}}$	moist$_{\text{2ha, 10m}}$	lakes$_{\text{2ha, 100m}}$	stream expansion
dry$_{\text{30ha, 100m}}$	mesic-moist$_{\text{30ha, 10m}}$	wet$_{\text{2ha, 10m}}$	lakes$_{\text{30ha, 10m}}$	stream contraction
dry$_{\text{RZ:2ha, 10m}}$	mesic-moist$_{\text{30ha, 100m}}$	moist$_{\text{2ha, 100m}}$	lakes$_{\text{30ha, 100m}}$	stream density$_{\text{2ha}}$
dry$_{\text{RZ:2ha, 100m}}$	mesic-moist$_{\text{RZ:2ha, 10m}}$	wet$_{\text{2ha, 100m}}$	lakes$_{\text{RZ:2ha, 10m}}$	stream density$_{\text{10ha}}$
dry$_{\text{RZ:10ha, 10m}}$	mesic-moist$_{\text{RZ:2ha, 100m}}$	moist$_{\text{30ha, 10m}}$	lakes$_{\text{RZ:2ha, 100m}}$	stream density$_{\text{30ha}}$
dry$_{\text{RZ:10ha, 100m}}$	mesic-moist$_{\text{RZ:10ha, 10m}}$	wet$_{\text{30ha, 10m}}$	lakes$_{\text{RZ:10ha, 10m}}$	dry$_{\text{RZ:30ha, 10m}}$
dry$_{\text{RZ:30ha, 100m}}$	mesic-moist$_{\text{RZ:10ha, 100m}}$	moist$_{\text{30ha, 100m}}$	lakes$_{\text{RZ:10ha, 100m}}$	dry$_{\text{30ha, 10m}}$
	mesic-moist$_{\text{RZ:30ha, 10m}}$	wet$_{\text{30ha, 100m}}$	lakes$_{\text{RZ: 30ha, 10m}}$	
	mesic-moist$_{\text{RZ:30ha, 100m}}$	moist$_{\text{RZ:10ha, 100m}}$	lakes$_{\text{RZ:30ha, 100m}}$	
		wet$_{\text{RZ:2ha, 10m}}$		
		moist$_{\text{RZ:2ha, 100m}}$		
		wet$_{\text{RZ:2ha, 100m}}$		
		moist$_{\text{RZ:10ha, 10m}}$		
		wet$_{\text{RZ:10ha, 10m}}$		
		moist$_{\text{RZ:10ha, 100m}}$		
		wet$_{\text{RZ:10ha, 100m}}$		
		moist$_{\text{RZ:30ha, 10m}}$		
		wet$_{\text{RZ:30ha, 10m}}$		
		moist$_{\text{RZ:30ha, 100m}}$		
		wet$_{\text{RZ:30ha, 100m}}$		

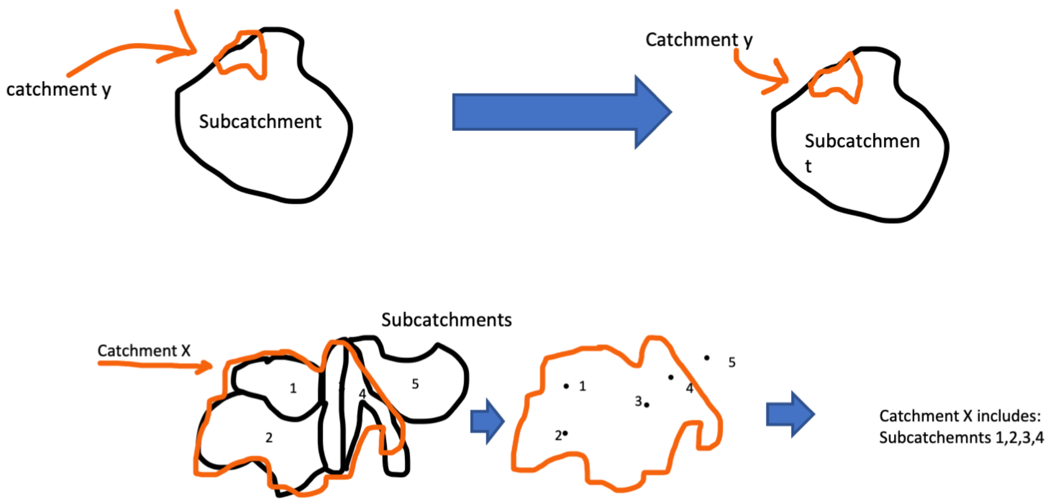
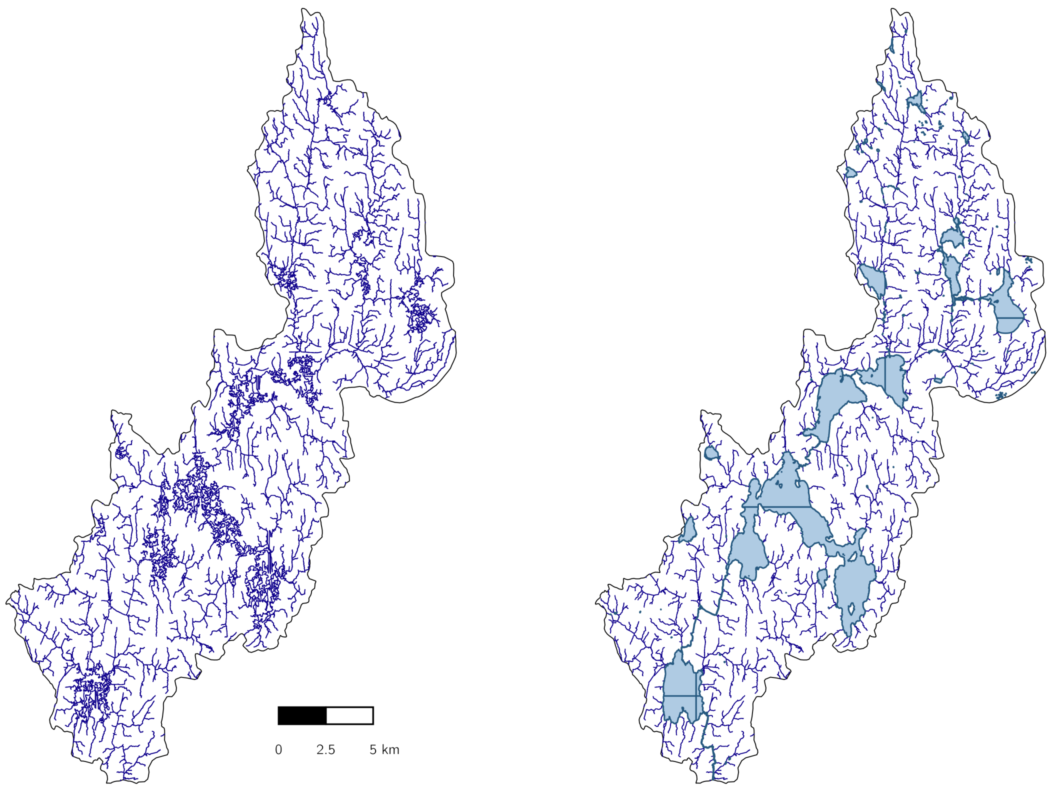


Fig. S1: Graphical representation of issues arising from inconsistencies in catchment boundaries. In the top line the small catchment with monitoring station reaches beyond the extent of the sub-catchment use for the FDS creation. The small catchment had to be trimmed to be within the sub catchment so that fringe effects of the creation of the FDS rasters were excluded. The lower line represents the creation of a dictionary that gives which sub-catchments make up the catchment with monitoring station based on a point on surface method.



(a)

(b)

Fig. S2: Modeled stream network at 10ha stream initiation size from LiDAR data forms a chaotic line system where there is open water as the software is unable to deal with open water (a). Therefore open water of the swedish property map is used to eliminate random lines, however, this is not perfect and leaves behind some lines (b).

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