

High-resolution modelling of dissolved organic carbon dynamics in a boreal nested catchment: insights from the Krycklan-HYPE model

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ABSTRACT

Understanding the spatiotemporal dynamics of dissolved organic carbon (DOC) is essential for predicting aquatic carbon fluxes and managing water quality in boreal catchments. Traditional DOC modelling approaches are limited in their ability to represent seasonal dynamics, event-driven responses, and riparian-zone contributions. Here, we evaluate the performance of the Krycklan-HYPE model in simulating streamflow and DOC concentrations across the Krycklan catchment in northern Sweden. The model was calibrated and validated for 14 sub-catchments using the Kling-Gupta Efficiency (KGE) metric. Results showed consistently good to very good performance for streamflow (calibration KGE = 0.50–0.82; validation KGE = 0.35–0.71), with low uncertainty and strong spatial transferability. In contrast, the success of DOC simulations was more varied, with KGE values across streams of 0.11–0.59 for the calibration period and 0.05–0.58 for the validation period (excluding one negative value). A negative correlation between streamflow simulation performance and DOC simulation performance was observed, indicating a trade-off between hydrological and biogeochemical simulation accuracy. Seasonal analysis showed that streamflow and DOC were best captured during spring and autumn, while DOC dynamics during summer and high-flow events were not well simulated. This pointed to the model structure limitation with missing representations of corresponding processes. Scenario-based analysis further highlighted that streamflow was best simulated under high flows, while DOC performance was better under low flow conditions. These results demonstrate the Krycklan-HYPE model's strengths in streamflow simulation but also underscore limitations in representing DOC mobilization and transport. Future studies should focus on developing model structures that incorporate relevant processes, and adopting calibration strategies that account for spatially heterogeneous parameterization.

1. Introduction

Dissolved organic carbon (DOC) plays a critical role in the global carbon cycle, linking terrestrial and aquatic environments. Inland waters receive a substantial portion of the Earth's terrestrial net ecosystem production, with an estimated land-to-water export of approximately 5.1 Pg of carbon annually (Drake et al., 2018; Soares et al., 2019). Of this, around 20% is transported through the freshwater network to the ocean (Senatore et al., 2023), with over 50% of this transport occurring in the form of DOC (Chaplot & Mutema, 2021; Cole et al., 2007). Beyond its critical role in the carbon cycle, DOC considerably influences water

quality and aquatic ecosystem health. For instance, DOC can enhance the mobility of harmful contaminants, such as heavy metals, through complexation processes (Lawlor & Tipping, 2003), with potential risks to human health (Chowdhury et al., 2009). In aquatic ecosystems, DOC regulates key processes, including light penetration, primary production, and the bioaccumulation of methyl mercury in food webs (Mukundan et al., 2023).

In recent decades, DOC concentrations in surface waters have risen rapidly across the Northern Hemisphere (de Wit et al., 2021; Garmo et al., 2014; Monteith et al., 2007), with far-reaching implications for aquatic ecology, ecosystem services, and the global carbon balance.

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Seasonal hydrological dynamics have been identified as key drivers of DOC export. For instance, more than 50% of dissolved carbon export occurs during spring, while rainfall events during the growing season contribute an additional 40% (Tong et al., 2024). Hydroclimatic events can further disrupt organic matter decomposition and enhance DOC mobilization from soils to streams (Senatore et al., 2023; Wu et al., 2023). Given these complex interactions, improving our understanding and prediction of DOC dynamics is essential for advancing carbon cycle science, mitigating climate impacts, and maintaining ecosystem functions.

Computational models provide a powerful method of studying DOC dynamics at spatial and temporal scales not possible with field monitoring alone. While in-situ measurements offer valuable insights, their spatial and temporal coverage is limited. Models can integrate multiple data sources and are particularly valuable for simulating DOC fluxes under changing climatic and land-use conditions. Among different modelling approaches, process-based models are widely used because they represent key physical and biogeochemical processes. Examples include the Integrated Catchment model for Carbon (INCA-C), which integrates carbon biogeochemistry with hydrological flow paths (Oni et al., 2012), and the extension of the Soil and Water Assessment Tool (SWAT), SWAT-Carbon, which incorporates carbon cycling and DOC transport processes (Du et al., 2019; Qi et al., 2020).

Despite these advances, existing DOC models have limitations. For instance, INCA-C has difficulty in capturing the effects of drought duration and severity on DOC timing and magnitude, and does not represent riparian zones (Futter et al., 2007; Futter et al., 2011; Sharma et al., 2023; Wu et al., 2024). SWAT-Carbon has demonstrated sensitivity to climate input resolution and often underestimated streamflow and DOC loads during short, intense storm events, particularly in wet regions where its bucket-based soil moisture scheme limits performance (Du et al., 2023; Du et al., 2020b; Du et al., 2019; Qi et al., 2018).

The Hydrological Predictions for the Environment (HYPE) model, developed by the Swedish Meteorological and Hydrological Institute (SMHI), is a semi-distributed, process-based model designed to simulate hydrology and water quality (Lindström et al., 2010; Pers et al., 2016). Building on the HBV ("Hydrologiska Byråns Vattenbalansavdelning" model) framework, HYPE incorporates flexible spatial discretization and flow-path partitioning, which in principle allow the representation of varied landscape units. Its modular structure includes a riparian-zone process intended to represent the riparian influence on DOC. HYPE has been applied to simulate hydrological processes and nutrient dynamics (e.g., nitrogen and phosphorus) across diverse climatic and physiographic conditions, from small catchments to continental and global applications (Arheimer et al., 2012b; Capell et al., 2021; Chen et al., 2024; Donnelly et al., 2016; Du et al., 2020a; Ghaffar et al., 2021; Namugize et al., 2017; Phillips et al., 2024; van Vliet et al., 2015; Woldegiorgis et al., 2023; Wynants et al., 2024; Yin et al., 2016).

The DOC module was first introduced in the Swedish national application of the HYPE model (S-HYPE) by Pers et al. (2016), who demonstrated its potential to represent broad spatial patterns in DOC concentrations at the national scale. However, evaluation of DOC performance of HYPE has remained limited since its initial development. In particular, systematic evaluation of DOC dynamics across nested catchments is largely absent from the literature. Most subsequent HYPE applications have focused on hydrology or nutrient transport, leaving open questions about the model's ability to reproduce DOC mobilization and transport processes across spatial scales and hydrological conditions.

Boreal catchments store approximately one-third of the Earth's terrestrial carbon, primarily in soils and peatlands (Merilä et al., 2024; Pan et al., 2011), and are particularly sensitive to environmental changes. DOC represents a dominant pathway for carbon transfer from terrestrial to aquatic systems in these regions, influencing both regional and global carbon budgets. Climate change is altering DOC dynamics in these catchments, where rising temperatures and shifting hydrological

patterns enhance DOC mobilization from soils to aquatic networks (Bowering et al., 2023; Roebuck Jr et al., 2023). The Krycklan catchment in northern Sweden represents one of the most well-instrumented boreal catchments for DOC studies (Laudon et al., 2013). With extensive monitoring across its nested sub-catchments since the 1980s, Krycklan provides a unique dataset for model development and evaluation. Previous DOC modelling efforts in Krycklan include empirical and hybrid approaches: Kasurinen et al. (2016) highlighted the importance of soil moisture using an empirical model across 18 sub-catchments; Oni et al. (2015) assessed clear-cut impacts on DOC by coupling empirical and process-based models; and Liu et al. (2024) investigated the influence of wetland impoundments on DOC transport in wetland-dominated sub-catchments.

By leveraging the nested structure of Krycklan, this study introduces the Krycklan-HYPE model, developed specifically for streamflow and DOC simulations in 14 sub-catchments of the Krycklan catchment. This allows evaluation of model performance from small headwaters to the full catchment and provides a more comprehensive assessment of spatial and seasonal variability in DOC dynamics than studies focused on individual sub-catchments. It serves as a robust testbed for refining DOC process representation within HYPE. Moreover, given SMHI's plans to simulate riverine DOC for all major Swedish rivers using HYPE, insights gained from Krycklan can guide upscaling of DOC simulations to larger boreal regions or national applications, supporting improved carbon budget assessments.

Specifically, objectives of this study are to: (1) set up and calibrate the Krycklan-HYPE model for daily streamflow and DOC simulations; (2) evaluate the model's performance and uncertainty in simulating streamflow and DOC; and (3) investigate seasonal variability in model performance and analyse model sensitivity to different scenarios.

2. Study area

The Krycklan catchment, located approximately 50 km northwest of Umeå in northern Sweden (64°14'N, 19°46'E), covers an area of 68 km² and represents one of the most intensively studied boreal research sites (Fig. 1). The catchment is part of the Svartberget field research infrastructure, managed by the Swedish University of Agricultural Sciences (SLU) (Laudon et al., 2013). Krycklan features elevations ranging from 114 to 405 m above sea level. The land cover is predominantly forested (87%), dominated by Scots pine and Norway spruce, with wetlands, primarily oligotrophic mires, covering significant areas in some sub-catchments. The region experiences a cold temperate humid climate, with a mean annual temperature of 1.8°C and annual precipitation of 614 mm, approximately 35–50% of which falls as snow. Snow cover persists for about 167 days annually, with peak runoff occurring during the spring snowmelt period (April–May) (Laudon et al., 2021; Zhu et al., 2024). The catchment has been a focal study site for long-term multi-disciplinary environmental research since 1980, and provides valuable insights into hydrological and biogeochemical dynamics, as well as forest ecology, and climate change impacts on boreal ecosystems.

3. Data and methods

3.1. Data

This study utilized data from multiple sources to achieve its objectives (Table 1). Daily meteorological measurements (mean, maximum, and minimum temperature, and precipitation) were obtained from the Svartberget station, part of the Swedish Infrastructure for Ecosystem Science (SITES. Svartberget Research Station, 2025). Streamflow and DOC concentration data were collected for each sub-catchment from SITES, with streamflow recorded daily and DOC sampled frequencies ranging from biweekly to several times per week (Laudon et al., 2013). While meteorological data were consistent across all sub-catchments, streamflow and DOC measurements were site-specific, and their

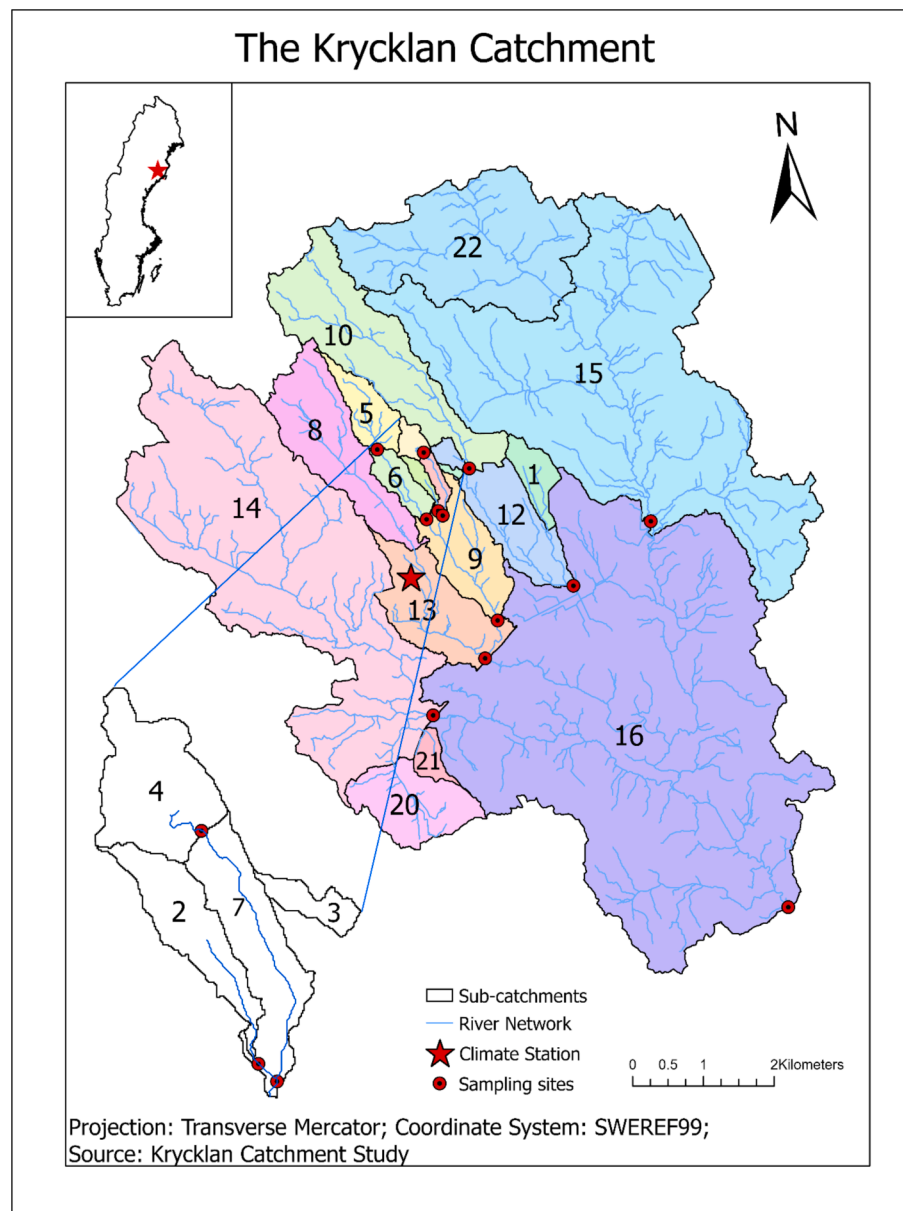


Fig. 1. The Krycklan catchment and its conventionally numbered sub-catchments. Sub-catchments are referred to in the text using the prefix “C” (e.g., C01 and C02 corresponding to the map labels 1 and 2, respectively).

temporal coverage varied due to differences in infrastructure installation and monitoring capacity. Additional datasets included a 2-meter resolution Digital Elevation Model from the SLU Geodata Portal (SLU, 2025), SMHI reclassified soil data from the Swedish Geological Survey (SGU), land use data from the National Land Cover Data (NMD), and a humus carbon map from SLU.

3.2. HYPE model

The HYPE model family follows a naming convention that reflects geographic scope and regional representation. For example, S-HYPE refers to the national-scale HYPE model for Sweden (Strömqvist et al., 2012), E-HYPE represents the European-scale application of HYPE (Donnelly et al., 2013), and Balt-HYPE refers to the Baltic Sea basin setup (Arheimer et al., 2012a). Following this tradition, we refer to the HYPE model applied in this study as Krycklan-HYPE, designed for hydrological and DOC simulations in the Krycklan catchment, calibrated and validated for its 14 sub-catchments.

HYPE divides the study area into sub-catchments, which are further subdivided into Soil-Land-use Classes (SLCs). Each SLC contains three soil layers of varying thickness and represents the smallest computational unit. The model is driven by temperature and precipitation data (daily or hourly) and simulates hydrological and biogeochemical processes at the SLC level, before aggregating results to the sub-catchment and catchment scales. For process flexibility, HYPE offers a range of algorithm options. For example, five methods are available for simulating potential evapotranspiration, including the modified Jensen-Haise/McGuinness method, the modified Hargreaves-Samani method. Here we applied the modified Hargreaves-Samani method. Calibration can be performed against multiple observations such as snow water equivalent, groundwater levels, and streamflow. Detailed descriptions of the model's equations and processes are available on the HYPE Wiki page (<https://hype.smhi.net/wiki/doku.php>) and supporting literature (Lindström et al., 2010; SMHI, 2024).

Table 1

Data used in this study.

Type	Data	Unit	Source
Meteorological data	mean temperature	°C	SITES – Svartberget station (https://meta.fieldsites.se/resources/stations/Svartberget)
	precipitation	mm/day	
	Maximum temperature	°C	
Observed data	Minimum temperature	°C	SLU geodata (https://www.slu.se/bibliotek/soka-lana/soka/sok-digitala-kartor-och-geodata/)
	DOC concentration	mg C/L	
	Daily discharge	m ³ /s	
Geographical data	DEM	m	SMHI (https://www.smhi.se/data/sjoar-och-vattendrag/vattenwebb/om-data-i-vattenwebb/indata-for-jordarter-i-vattenwebb)
	Soil type	–	
	Land use	–	
	Humus carbon	kg C/ha	SLU (https://www.slu.se/en/environmental-data/environmental-data-catalogue/maps-carbon-stock-and-carbon-stock-change-in-swedish-soils/)

3.2.1. Rainfall-runoff processes

HYPE simulates major processes of the water cycle, including snow accumulation and melt, evapotranspiration, infiltration, percolation, surface runoff, and subsurface flow. Precipitation is partitioned into rain and snow based on temperature threshold, and snowmelt is calculated using a temperature-index approach, with optional module to account for radiation and snow cover effects.

A portion of precipitation infiltrates into the upper soil layer, limited by a maximum infiltration rate (*mactrinf*), which varies by soil type. When soil moisture exceeds a macropore flow threshold (*mactrsm*), excess water contributes to macropore flow, governed by a soil-specific runoff coefficient (*macrate*). Another fraction of precipitation is converted into surface runoff via a soil-specific coefficient (*srrate*), while any remaining precipitation enter a surface water pool and is released as overland flow according to a land use-specific recession coefficient (*srrcs*). Evapotranspiration is assumed to occur from the two upper soil layers. Actual evapotranspiration equals to evapotranspiration (PET) when soil moisture exceeds a defined proportion (*lp*) of field capacity; below this threshold, actual evapotranspiration declines linearly to zero at the wilting point. Runoff from the soil zone occurs when soil moisture exceeds field capacity, governed by recession coefficients (*rrcs*). Percolation occur when the upper layer exceeds field capacity, with rates determined by a parameter (*mperc*). Groundwater levels are estimated based on soil zone saturation, particularly where pore spaces are fully filled.

3.2.2. DOC processes

DOC dynamics from terrestrial to aquatic ecosystems are simulated through coupled hydrological transport and biogeochemical transformation processes. The model simulates DOC from decomposing plant material through temperature- and moisture-dependent transformations in soils, and subsequent transport to aquatic systems through surface and subsurface flows. The structure captures the coupled physical and biological controls on DOC fluxes across spatial scales from individual soil layers to entire catchments (Pers et al., 2016).

3.2.2.1. Soil carbon pools and initialization. The model represents soil organic carbon through three interacting pools within each soil layer. The fast turnover carbon pool (*fastC*) contains labile organic carbon from recent plant residues including leaf litter, crop debris, and root exudates. The slow turnover carbon pool (*humusC*) stores more recalcitrant organic carbon with decadal turns over times, supplying DOC through gradual dissolution. The DOC pool represents the mobile fraction in soil water, linking terrestrial carbon to aquatic export via hydrological transport. Initial carbon pool sizes are determined by land use and soil characteristics, with layer-specific values specified through model initialization parameters.

3.2.2.2. Soil carbon transformations. In soil, four key processes govern transfers between carbon pools, all modulated by soil temperature dependence factor (*tmpfcn*) and soil moisture dependence factor (*smfcn*) (Lindström et al., 2010; Pers et al., 2016). The first process is the transformation of *fastC* to *humusC* (*fasttohumus(k)*, mg/m²/day), which occurs primarily in the top soil layer. In deeper layers, this transformation includes a mineralization fraction. The second process is DOC generation through the turnover of *fastC* (*transfC(k)*, mg/m²/day). The third is DOC generation from the turnover of *humusC* (*transhC(k)*, mg m²/day). And the forth process is DOC immobilization back into *fastC* (*DOCtofastC(k)*, mg/m²/day), which occurs when soil temperature is below 5°C and soil moisture indicates dry conditions:

$$fasttohumus(k) = klh \times tmpfcn(k) \times smfcn(k) \times fastC(k), k = 1 \quad (1)$$

$$fasttohumus(k) = klh \times tmpfcn(k) \times smfcn(k) \times fastC(k) \times (1 - minc), k = 2, 3 \quad (2)$$

$$transfC(k) = klo \times tmpfcn(k) \times smfcn(k) \times fastC(k) \times (1 - minc), k = 1 \dots 3 \quad (3)$$

$$transhC(k) = kho \times tmpfcn(k) \times smfcn(k) \times humusC(k) \times (1 - minc), k = 1 \dots 3 \quad (4)$$

$$DOCtofastC(k) = kof \times DOC(k) \times (1 - minc), k = 1 \dots 3 \quad (5)$$

where *k* is the soil layer, *minc* is the proportion of mineralization, *klh* is a vegetation-dependent parameter, and *klo*, *kho*, and *kof* are general parameters, *DOC(k)* (mg/m²) is the soil DOC pool.

3.2.2.3. Hydrological transport mechanisms. DOC moves through the landscape via three interconnected pathways: (i) moves vertically between soil layers through percolation, (ii) flow laterally towards stream, (iii) riparian zone processing, (iv) flow in streams and lakes.

Vertical percolation (*DOC_{Perc}*, mg/m²) transports DOC downward through the soil profile:

$$DOC_{Perc} = DOC(k) \times (1 - koc \times tmpfcn(k) \times smfcn(k)), k = 1 \dots 3 \quad (6)$$

where *koc* is a general parameter for percolation between soil layers.

DOC in lateral runoff passes through a temporary DOC pool (*relpool*, mg/m²) before it is transported to river stream. The DOC stored in this temporary pool is released and routed to the river as a function of total runoff (*runoff*, mm ts⁻¹, ts means time step, in this study is day):

$$relpool = relpool + runoffC \quad (7)$$

$$release = \min(relpool, relpool \times (runoff/ocfldelx)^{ocfdele}) \quad (8)$$

where *runoffC* (mg/m²) is the sum of DOC from surface runoff, soil layer runoffs and tile drainage. *release* (mg/m²) is the available DOC for transport to river streams. *ocfldelx* and *ocfdele* are general parameters.

The riparian zone is the final terrestrial process before lateral runoff enters streams, which increases DOC concentration with a factor $f(k)$ and maintain flow volume:

$$f(k) = 1 + \text{ripz} \times \text{tempfcn}(k) \times \left(\frac{\text{elev}}{1000} \right) \times f_{\text{grw}} \times f_{\text{season}} \times f_{\text{sm}}, k = 1 \dots 3 \quad (9)$$

$$\text{conc}(k) = f(k) \times \text{conc}(k), k = 1..3 \quad (10)$$

$$f_{\text{grw}} = e^{\text{ripe} \times \text{gwat}} \quad (11)$$

$$f_{\text{season}} = \begin{cases} \text{rips, autumn} \\ 1, \text{otherwise} \end{cases} \quad (12)$$

$$f_{\text{sm}} = \begin{cases} 0, \text{sm} \leq \text{wp} \\ f_2(\text{sm}), \text{wp} < \text{sm} < \text{pw} \\ \text{satact}, \text{sm} \geq \text{pw} \end{cases} \quad (13)$$

$$f_2(\text{sm}) = \begin{cases} \min \left(1, \text{satact} + \frac{(1 - \text{satact}) \times \text{pw} - \text{sm}}{d \times \theta_{\text{upp}}}, \frac{\text{sm} - \text{wp}}{d \times \theta_{\text{low}}} \right), \text{rising grw} \\ \min \left(1, \text{satact} + \frac{(1 - \text{satact}) \times \text{pw} - \text{sm}}{d \times \theta_{\text{upp}}}, \frac{\text{satact} \times \text{sm} - \text{wp}}{d \times \theta_{\text{low}}} \right), \text{sinking grw} \end{cases} \quad (14)$$

where *elev* is altitude, f_{grw} , f_{season} , and f_{sm} are groundwater-, season-, and soil moisture- dependent functions. The *ripz* is a land use dependent parameter, *ripe* is a groundwater level dependent parameter, and *rips* is a parameter dependent on the season. Moreover, $\text{conc}(k)$ is the DOC concentration in runoff of each soil layer. The autumn is determined when ten-day mean temperature is lower than twenty-day mean temperature. θ_{upp} and θ_{low} are coefficients, *satact* is the saturation parameter. Finally, *sm* is soil moisture, *wp* is the wilting border and *pw* is the total pore volume, in fractions of total soil layer thickness *d*.

During flows in streams and lakes, DOC dynamics in rivers and lakes were simulated through balanced production and consumption (*minprodCpot*). Initial organic carbon concentrations in rivers are assumed to be zero, while lake concentrations are user-defined. Potential carbon transformation is calculated from potential nitrogen transformation (*minprodNpot*):

$$\text{minprodCpot} = \text{minprodNpot} \times \text{Nratio} \quad (15)$$

$$\text{minprodNpot} = \text{wprod} \times \text{TPfcn} \times \text{tmpfcn} \times \text{area} \times \text{depth} \quad (16)$$

Phosphorus dependence follows half-saturation kinetics (*TPfcn*) using long-term average total phosphorus concentrations. When phosphorus is not modeled by HYPE, a lake-dependent parameter (*tpmean*) is used to replace *TPfcn* instead:

$$\text{TPfcn} = \frac{(\text{TPconc} - \text{lmsedPP})}{(\text{TPconc} - \text{lmsedPP} + \text{halfsatTPwater})} \quad (17)$$

$$\text{tmpfcn} = \text{tmpfcn1} \times \text{tmpfcn2} \quad (18)$$

$$\text{tmpfcn1} = \frac{\text{watertemp}}{20} \quad (19)$$

$$\text{tmpfcn2} = \frac{(T_{10} - T_{20})}{5} \quad (20)$$

where *wprod* is the production and decay parameter, *area* is lake area, *depth* is water depth, *lmsedPP* is a general parameter, *Nratio* is the

carbon–nitrogen ratio, *watertemp* is water temperature, T_{10} and T_{20} are the ten-day and twenty-day mean air temperatures.

Lake sedimentation ($\text{sedC}_{\text{lake}}$) is calculated by:

$$\text{sedC}_{\text{lake}} = \text{sedoc} \times \text{conc} \times \text{area} \quad (21)$$

where *area* is lake area, *conc* is DOC concentration in lakes, and *sedoc* is a general parameter.

3.2.3. Model calibration and validation

Model calibration and validation were conducted using observed daily streamflow and DOC concentration data from 14 sub-catchments. A two year warm-up (2009–2010) was applied prior to calibration to minimize the influence of initial conditions on model state variables. Subsequently, it was calibrated for the period 2011–2015 and validated independently for 2016–2020. The objective function for calibration was defined as a combination of two Kling-Gupta Efficiency (KGE) values, representing streamflow (KGE_Q) and DOC (KGE_{DOC}), with equal weights of 0.5 assigned to each:

$$f = 0.5 * KGE_Q + 0.5 * KGE_{\text{DOC}} \quad (22)$$

The KGE values were calculated as:

$$KGE = 1 - \sqrt{(r - 1)^2 + \left(\frac{\sigma_{\text{sim}}}{\sigma_{\text{obs}}} - 1 \right)^2 + \left(\frac{\mu_{\text{sim}}}{\mu_{\text{obs}}} - 1 \right)^2} \quad (23)$$

where *r* is the linear correlation between observed and simulated values. σ_{sim} and σ_{obs} are the standard deviations of simulated and observed values, respectively, μ_{sim} and μ_{obs} are the mean simulated and observed values, respectively.

Following the approach of Hundecha et al. (2016), who applied the HYPE model to simulate daily streamflow across Europe, we employed the Monte Carlo method with 10,000 iterations for calibration. All of the calibrated parameters and their initial ranges are summarized in Table 2:

3.3. Model evaluation and uncertainty analysis

In addition to selecting the best parameter set for calibration and validation analysis, the 100 best parameter sets (selected from 10000 runs) were used to assess the model uncertainty. This approach filters out parameter sets that produce unrealistic simulation (e.g., negative KGE value for DOC although total KGE behave good) while retaining simulations that reflect acceptable model behaviours (Guo et al., 2024; Mohammadi et al., 2023). In addition to the multi-objective function, we calculated individual KGE values for streamflow and DOC, as well as the coefficient of determination (R^2) and correlation coefficient (*r*). KGE performance was classified as “good” ($KGE \geq 0.75$), “satisfactory” ($0.75 > KGE \geq 0.5$), and “poor” ($KGE < 0.5$) (Bisselink et al., 2016; Guo et al., 2024; Towner et al., 2019). Calibration uncertainty was assessed using the 95% prediction uncertainty (95PPU), derived from the 2.5th (X_L) and 97.5th (X_U) percentiles of the cumulative distribution of model outputs (Abbaspour et al., 2004; Abbaspour et al., 2007). The 95PPU represents the range within which 95% of simulated values are expected to fall.

Table 2

Key parameters and the used range for calibration in the Krycklan-HYPE model.

Parameters	Unit	Definition	Range
wcfc	–	fraction of soil available for evapotranspiration	[0.05, 0.5]
wcwp	–	wilting point as a fraction	[0.05, 0.5]
wcep	–	effective porosity as a fraction	[0.05, 0.5]
mperc	mm ts ⁻¹	maximum percolation capacity from soil layer	[5, 120]
trrcs	ts ⁻¹	recession coefficient for tile drains	
rrcs	ts ⁻¹	recession coefficient for soil layer	[0.05, 0.6]
macrate	–	fraction for macro-pore flow	[0.05, 0.5]
mactrinf	mm ts ⁻¹	threshold for macro-pore flow	[0, 100]
mactrsm	–	threshold soil water for macro-pore flow and surface runoff	[0, 1]
macrofilt	–	filtration of PartP with macropore flow	[0, 1]
sracs	ts ⁻¹	recession coefficient for surface runoff	[0.01, 0.2]
cevp	mm °C ⁻¹	evapotranspiration parameter	[0.15, 0.3]
cmlt	mm ts ⁻¹	melting parameter for snow	[1, 4]
sracs	ts ⁻¹	fraction for surface runoff	[0.01, 0.5]
pcluse	–	correction factor for precipitation	[0, 0.3]
ttmp	°C	threshold temperature for snow melt, snow density and evapotranspiration	[-1, 1]
sracs	ts ⁻¹	recession coefficient for surface runoff	[0.01, 0.2]
surfmem	days	upper soil layer soil temperature memory	[0, 20]
depthrel	m ⁻¹	depth relation for soil temperature memory	[0, 5]
ocfldelx	mm ts ⁻¹	parameter for delay of OC from runoff	[1, 20]
ocfldele	–	parameter for delay of OC from runoff	[1.3, 2]
klh	d ⁻¹	parameter for speed of transformation from fastC to humusC in soil	[1*10 ⁻⁸ , 0.1]
klo	d ⁻¹	parameter for speed of transformation from fastC to OC in soil water	[1*10 ⁻⁸ , 0.1]
kho	d ⁻¹	parameter for speed of transformation from humusC to OC in soil water	[0.001, 0.1]
kof	d ⁻¹	parameter for speed of transformation from OC in soil water to fastC	[1*10 ⁻⁸ , 0.1]
koflim	–	parameter for threshold for wetness for transformation OC in soil water to fastC	[0, 0.85]
koc	–	parameter for DOC-concentrations reduction for percolation	[0, 1]
ripe	m ⁻¹	exponent for groundwater depth dependence of OC processes in riparian zones	[0, 20]
rips	–	seasonal factor for OC processes in riparian zones	[0, 20]
minc	–	fraction of transformation mineralised to inorganic carbon	[0, 0.2]
wprodc	Kg m ⁻³ d ⁻¹	production/decay of OC in water	[0, 1]
sedoc	m ts ⁻¹	sedimentation rate OC in lakes.	[0, 0.5]
occonc0	mg L ⁻¹	starting value, organic carbon concentration in soil	[0, 50]
ripz	–	parameter for OC processes in riparian zone	[0, 3]
fastc	mg m ⁻³	starting concentration for fastC pool in soil layers	[0, 5000]
mperc	mm ts ⁻¹	maximum percolation capacity from soil layers	[5, 120]

Note: Unit ts means time step, which in this study is day.

Two metrics were used to evaluate uncertainty: P-factor and the R-factor. The P-factor indicates the proportion of observed data enclosed within the 95PPU band, calculated as:

$$Pfactor = \frac{C}{N} * 100 \quad (24)$$

where N is the total number of data, C is the number of simulations falling within the 95PPU band, determined by:

$$C = count(X_{sim}^i \leq X_U^i \& X_{sim}^i \geq X_L^i), i = 1 \dots k \quad (25)$$

The R-factor, calculated as the ratio of the average width of the 95PPU band to the standard deviation of the observed data, reflects the thickness of the uncertainty interval. Lower R-factor values indicate narrower and more precise uncertainty bands. The R-factor is calculated as:

$$Rfactor = \frac{\overline{d_x}}{\sigma_x} \quad (26)$$

where σ_x is the standard deviation of measurements, and $\overline{d_x}$ is the average distance between X_L and X_U , calculated as:

$$\overline{d_x} = \frac{1}{k} \sum_{i=1}^k (X_U - X_L)_i, i = 1 \dots k \quad (27)$$

A P-factor close to 1 and an R-factor near 0 indicate a well-calibrated model. In practice, P-factor between 80% and 100% combined with low R-factor relative to data variability are considered robust. These metrics ensure a balance between capturing observed data within the uncertainty range and maintaining a narrow prediction interval (Bonakdari et al., 2019; Swain & Patra, 2017).

Finally, seasonal variability was assessed using long-term monthly averages for 2011–2020. Spatial performance was evaluated across upstream, downstream sub-catchments, and the catchment outlet. Scenario-based analysis focuses on low and high flow conditions, defined by the 25th and 75th percentiles of model outputs within each sub-catchment.

4. Results and discussion

4.1. Model calibration and validation

In this section, results are presented using the best-performing parameter set from calibration. The Krycklan-HYPE model simulated seasonal streamflow with consistently good to very good performance across sub-catchments, as showed in Fig. 2 and Appendix 1, including C09 (upstream), C15 (downstream), and C16 (catchment outlet). These sub-catchments were selected to represent different hydrological locations within the catchment and to demonstrate model performance across spatial scales. During calibration period, KGE values ranged from 0.50 in sub-catchment C14 to 0.82 in C10, with all sub-catchments exceeding the 0.5 “good” threshold. Validation showed a modest decline, with KGE values ranging from 0.35 to 0.71, yet overall performance remained acceptable (Bisselink et al., 2016; Townner et al., 2019; Yuan et al., 2020).

Uncertainty analysis emphasized the robustness of the streamflow simulations. P-factors exceeded 80% across all sub-catchments in both calibration and validation periods, and often surpassed 90%, while R-factors remained relatively low (Appendix 5). These results indicate the model provides hydrological predictions that are both accurate and tightly constrained (Bonakdari et al., 2019; Phiri et al., 2021; Swain & Patra, 2017). The consistency across multiple sub-catchments and time periods suggests the Krycklan-HYPE model is well parameterized and exhibits strong spatial and temporal transferability of its hydrological components.

In contrast, DOC simulations were more varied and generally weaker than those of streamflow. Calibration KGE values ranged from 0.11 to 0.59, with C15 showing the best simulation (Fig. 3). Validation results declined further (0.05 to 0.58), with one negative KGE value (−0.1) in sub-catchment C13 (Appendix 3). This variability highlights the difficulty of consistently capturing DOC dynamics across heterogeneous sub-catchments (Jutebring Sterte et al., 2022). The lower temporal resolution of DOC measurements compared to streamflow may also have reduced calibration effectiveness and contributed to higher simulation uncertainty.

Uncertainty estimates for DOC further highlight these limitations. P-factors ranged from 40.8% to 100%, often accompanied by relatively

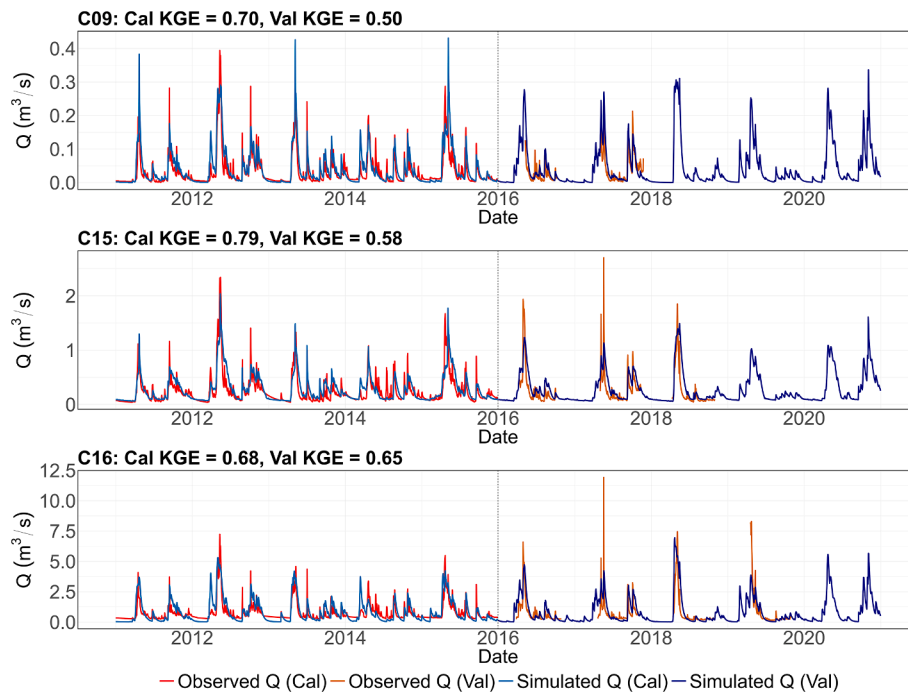


Fig. 2. Streamflow simulations for sub-catchments C09, C15, and the outlet C16. Cal represents calibration, Val represents validation.

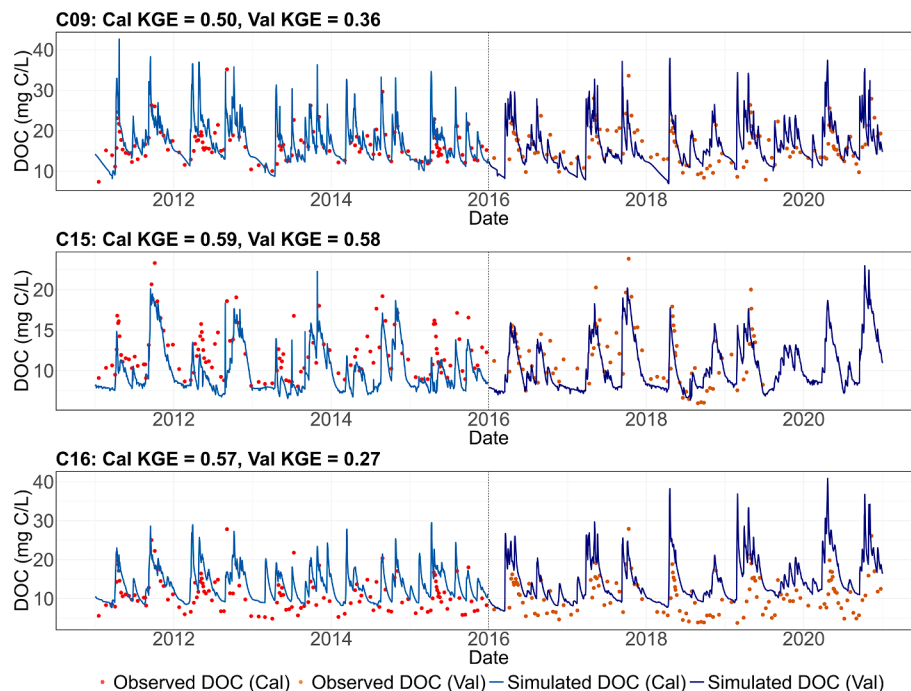


Fig. 3. DOC simulations for sub-catchments C09, C15, and the outlet C16. Cal and Val represent calibration and validation respectively.

high R-factors, suggesting that wide uncertainty bounds were often necessary to capture observed DOC concentrations. Since DOC is transported by water flow and the DOC module in HYPE builds upon the more mature rainfall-runoff module, strong streamflow performance would typically indicate a solid foundation for DOC simulation. However, the elevated uncertainty likely reflects the model's limited capacity to capture the complex and spatial variability of DOC mobilization.

Although Krycklan-HYPE performs well in simulating streamflow, and demonstrate consistent performance during the calibration and

validation periods, its DOC simulation performance appears more limited. The modest DOC performance may stem from both less targeted parameter optimization and structural model gaps that constrain its ability to simulate DOC production, mobilization, and transport, which are governed by fine-scale biogeochemical and hydrological interactions (Laudon et al., 2016; Reidy et al., 2025a; Reidy et al., 2025b).

One structural limitation may be that the model simplifies biogeochemical processes that influence DOC concentrations. For instance, the model does not explicitly account for sorption and desorption processes, which are critical for DOC retention and turnover in soils (Ågren et al.,

2007). While such interactions may be partly captured through the temporary DOC pool in soil and its delayed release, our approach does not reflect the dynamic controls exerted by soil mineralogy or organic matter content. Sorption has been shown to play a pivotal role in regulating the availability and mobility of DOC, especially in soils with high silt content and large specific surface areas, where increased mineral adsorption can enhance DOC mineralization and reduce concentrations (Kalbitz et al., 2000). Models such as DyDOC have demonstrated that DOC supply and turnover are highly dependent on sorption interactions, particularly within humic-rich soil layers (Michalzik et al., 2003; Mieres Dinamarca, 2016).

Calibration strategy also introduces challenges. In this study, a single, unified parameter set was applied across all sub-catchments to test the model's ability to reproduce DOC dynamics across Krycklan's heterogeneous landscape. This approach avoids overfitting and maintains model generality but means that local conditions such as wetland effects on DOC may not be well reflected in parameter values. As a result, some sub-catchments are better simulated than others, revealing the model's limited ability to generalize across diverse landscape conditions. A similar limitation was noted by Guo et al. (2024) when applying the FLEX model in the same Krycklan catchment, suggesting that achieving spatial consistency in DOC simulation is a persistent challenge in nested catchment modelling.

A key insight from the multi-objective model evaluation was the trade-off between streamflow and DOC performance. Across the top 100 parameter sets, a consistent negative correlation was observed between KGE values of the two variables (Fig. 4). Improving streamflow accuracy often reduced DOC performance, and vice versa.

The weak negative correlations between streamflow and DOC performance shown in Fig. 4 indicate that improved discharge simulation does not necessarily translate into improved DOC dynamics. This trade-off reflects structural limitations in how hydrological and biogeochemical processes are coupled in the model. In HYPE, DOC behaves as a reactive tracer whose mobilization and transport depend strongly on flow-path partitioning (e.g., shallow versus deeper subsurface contributions). Consequently, even when streamflow is well reproduced at the catchment outlet, the simulated distribution of contributing flow paths

may not correspond to those dominating DOC production and mobilization.

This is likely amplified by the simplified representation of soil processes in HYPE, which relies on only three soil layers for both saturated and unsaturated zones. Such a structure may be insufficient to capture the vertical heterogeneity of DOC production, storage, and release. In addition, inherent differences in streamflow and DOC dynamics further contribute to this trade-off. Hydrological responses during high-flow events are often difficult to simulate due to rapid fluctuations, whereas DOC concentrations during such events may follow more predictable mobilization and flushing patterns (Ågren et al., 2007; Laudon et al., 2004; Winterdahl et al., 2016). Conversely, baseflow conditions are more stable hydrologically but exhibit higher spatial and temporal variability in DOC due to complex subsurface processes.

4.2. Seasonal analysis

Seasonal evaluation reveals distinct performance patterns (Fig. 5). Streamflow was best simulated in spring and autumn, while DOC showed relatively better performance in these seasons compared to summer and winter, though deviations remained. The strong spring streamflow performance likely reflects the model's effective representation of snowmelt flow dynamics, which dominate runoff generation during this period. By contrast, summer and winter exhibited weaker performance, especially for DOC, which shows systematic error during summer, suggesting limitations in representing seasonally varying DOC mobilization processes.

This is further evidenced in Fig. 6, where observed DOC concentrations peak in summer—contrary to model predictions of a seasonal summer minimum for sub-catchments such as C02, C07 or C10 (Appendix 4). This mismatch arises from temperature- and precipitation-driven processes that are not explicitly represented in the model. Mean summer temperatures in Krycklan reach 13.6°C, roughly 11.6°C higher than in spring, and summer precipitation averages about 2 mm per day, the highest of any season (Appendix 7), increasing soil moisture and hydrological connectivity. Higher soil temperatures and increased acidity from intensified organic matter decomposition reduce

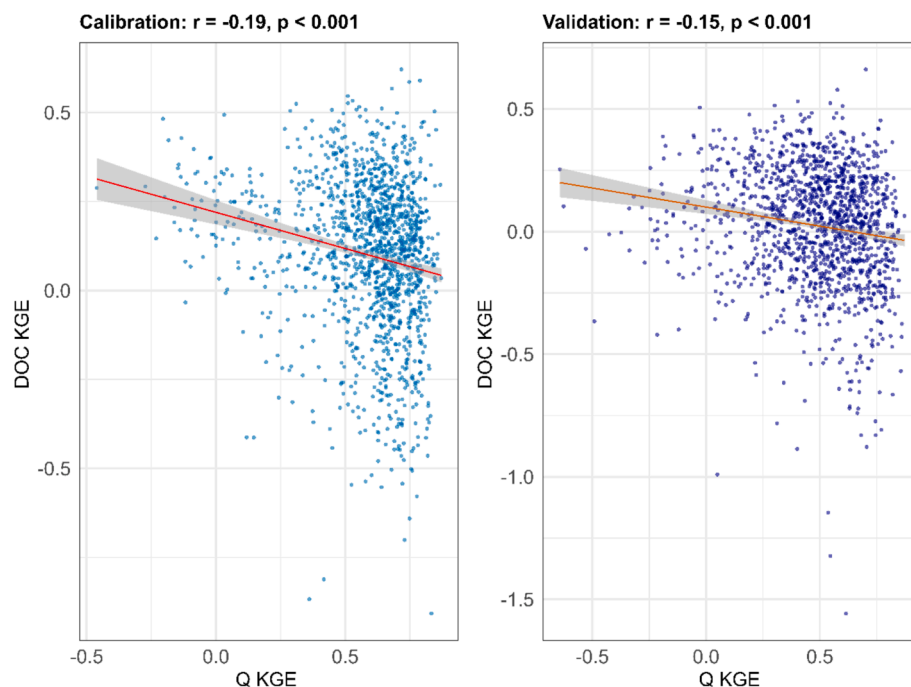


Fig. 4. The correlation between streamflow performance and DOC performance for the best 100 simulation across the entire catchment.

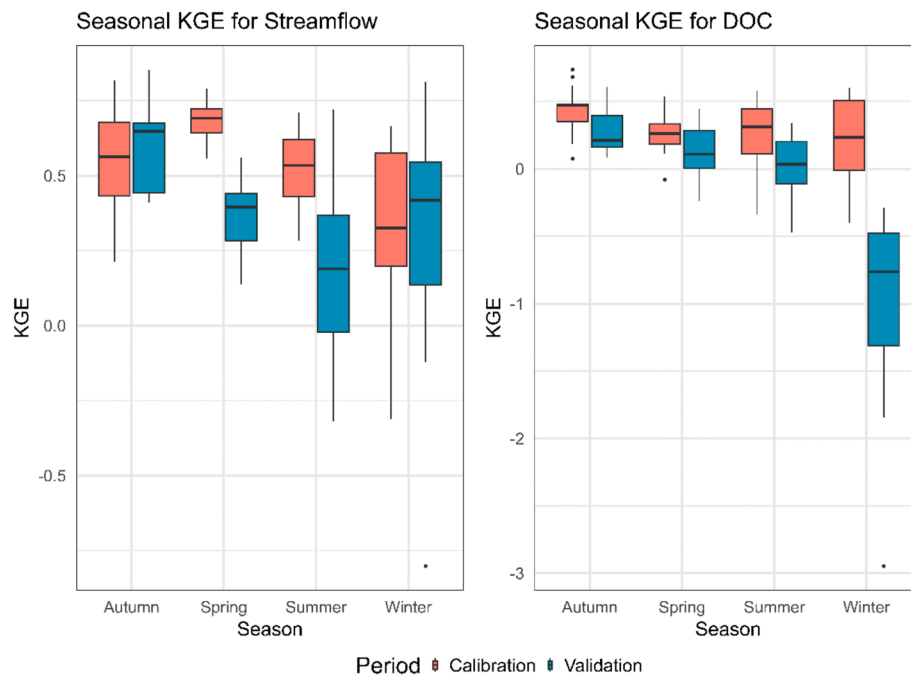


Fig. 5. The Krycklan-HYPE's seasonal performance across the entire catchment during calibration (2011–2015) and validation (2016–2020).

DOC sorption capacity (Kaiser et al., 2001). At the same time, intense precipitation events enhance soil moisture and hydrological connectivity, flushing DOC from shallow organic layers into streams (Dawson et al., 2008; Stutter et al., 2012). Furthermore, microbial mineralization intensifies in summer as warmer conditions stimulate heterotrophic microbial activity, enhancing the production of labile DOC fractions (Stutter et al., 2012). Microbial processing during warm, moist periods can generate rapid increases in dissolved organic matter, especially in riparian and upper organic soil layers (Köhler et al., 2008). Together, reduced sorption-driven retention, temperature-sensitive microbial DOC production, and precipitation-enhanced flushing, substantially elevate DOC availability and export during summer.

As the result, dry periods allow DOC buildup in soil porewaters due to microbial processing summer storm events flush accumulated DOC from soils into the streams (Raymond & Saiers, 2010). In such cases, even small variations in groundwater levels may trigger charge-release effects and episodic DOC transport, adding complexity that is difficult to predict, as stated in previous studies (de Wit et al., 2016; Warner & Saros, 2019; Wu et al., 2024). Together, reduced sorption, enhanced microbial DOC production, and hydrologically driven DOC flushing explain the pronounced summer DOC peaks observed in Krycklan help explain clarify why the current model consistently underestimates summer concentrations.

Additionally, in Krycklan, DOC source areas vary not only by flow conditions but also by landscape structure: during winter baseflow, DOC export is closely tied to wetland coverage, while spring snowmelt highlights the role of topography and catchment size. Prior work shows that in Krycklan, DOC sources shift seasonally, from wetlands under low-flow conditions to forested uplands during high flows, driven by the combined influence of hydrology and landscape connectivity (Ågren et al., 2007; Buffam et al., 2007; Laudon et al., 2011). Subcatchment C04 (Appendix 3, Appendix 6), with wetland coverage exceeding 50%, illustrates this complexity. While the model simulates DOC peaks during spring and autumn, similar to other sub-catchments, observed data show a distinctly different seasonal pattern: DOC remains at baseline levels during spring and winter, decline in summer, and increase sharply in autumn. This also suggests that some DOC processes or flow path interactions are not adequately represented by Krycklan-HYPE.

4.3. Scenario-based analysis

Performance under flow variability reveals contrasting behavior between streamflow and DOC (Figs. 7 and 8). High- and low-flow conditions were defined within each sub-catchment using the 75th and 25th percentiles. Streamflow was simulated more accurately during high-flows periods, with R^2 values up to 0.81, while low-flow conditions were less well captured. In contrast, DOC simulations showed better performance during low flows (calibration period: $R^2 = 0.36$; validation period: $R^2 = 0.29$), with weaker performance during high-flow DOC periods.

These contrasting trends reflect the model's strength and weakness. The model effectively represents hydrological processes dominant during high flows, such as surface runoff and rapid subsurface responses, as HYPE was initially developed for flood forecasting. DOC, however, is better represented under stable flow transport pathways and more stable biogeochemical conditions. This sensitivity to flow extremes aligns with existing literature emphasizing the importance of high-flow events in DOC export. For instance, Tong et al. (2024) showed that episodic storm events account for a disproportionate share of DOC export in forested catchments. Similarly, Senatore et al. (2023) reported that streamflow occurring during the highest 10% of discharge conditions contributed over 65% of total DOC yield in the Turbolo catchment, Italy (Senatore et al., 2023). Despite capturing streamflow dynamics, Krycklan-HYPE has limitations in simulating DOC responses during high-flow events.

Part of this mismatch between accurate simulation of streamflow during high-flow events and weaker representation of DOC dynamics under the same conditions is potentially attributed to the interplay of dilution and flushing processes, which varies across landscape types and sub-catchments. In wetland-dominated landscape such as sub-catchment C04, DOC concentrations commonly decline during the snowmelt discharge peak as meltwater bypasses organic-rich peat layers, leading to a dilution effect (Kasurinen et al., 2016; Rennermalm et al., 2010; Tiwari et al., 2019). In contrast, forested catchments exhibit a flushing pattern during high snowmelt and storm events: after dry periods, accumulated DOC in organic-rich surface soils is rapidly mobilized during rainfall, producing DOC peaks (Ågren et al., 2007; Laudon et al., 2011). However, Krycklan-HYPE does not distinguish these mechanisms across sub-catchments during spring, whereas

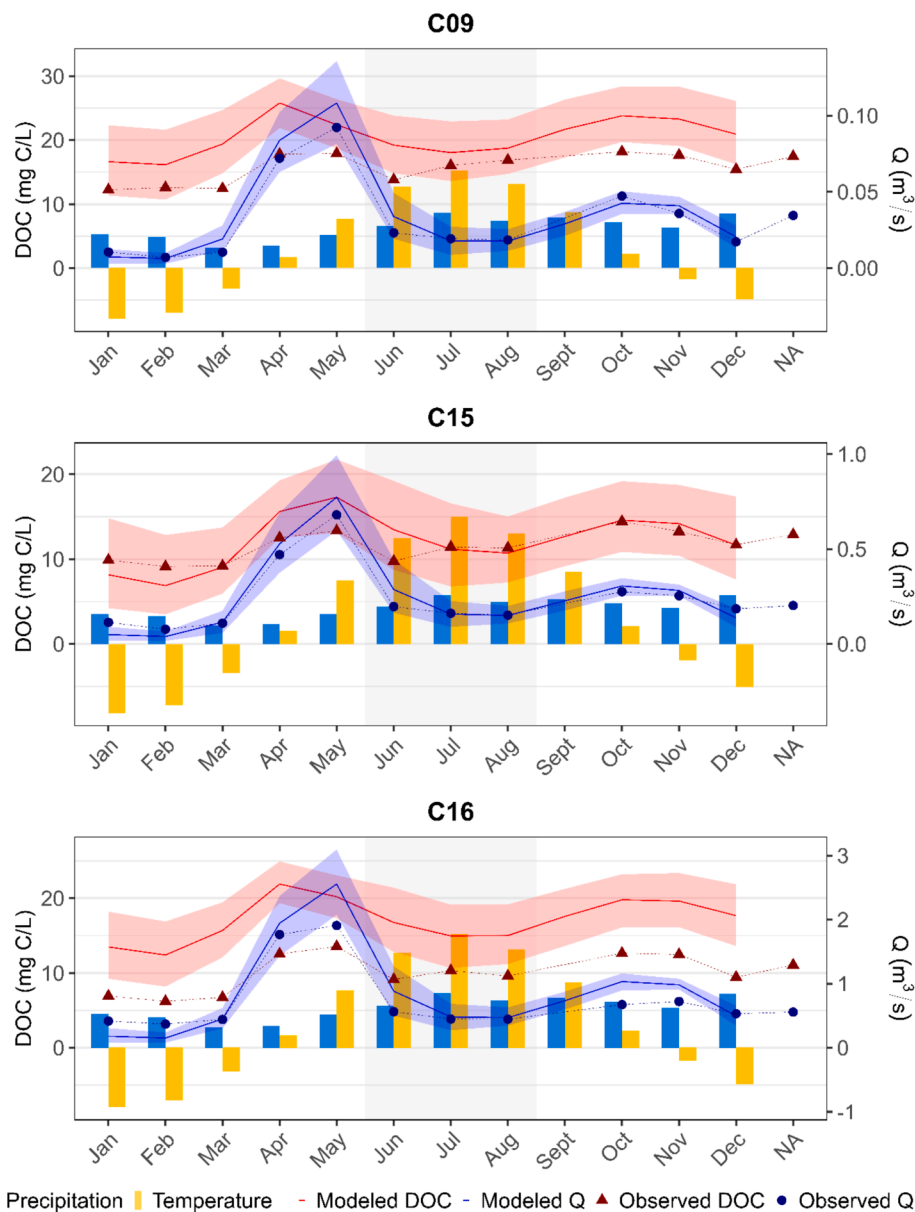


Fig. 6. Monthly streamflow and DOC dynamics during 2011–2020 of C09, C15 and C16. Monthly average temperature and precipitation during 2011–2020 are also shown. Summer months (Jun, July, August) are highlighted with grey background.

observations show distinctly different dilution and flushing patterns (Appendix 4).

A key structural gap underlying these patterns concerns groundwater and lateral subsurface flow representation. Krycklan-HYPE simulates a vertical soil water profile that accounts for both saturated and unsaturated zones, enabling partial representation of DOC mobilization during rising groundwater. This partially explains why DOC is reasonably captured during most low-flow periods, when transport is dominated by baseflow and relatively stable biogeochemical conditions. However, the model does not represent lateral groundwater flow between SLC classes, which becomes particularly important during high-flow events. Lateral subsurface pathways facilitate rapid DOC transport from organic-rich soils to streams, especially during intense summer storms or when shallow water tables increase hydrological connectivity (Wu et al., 2024). Water moving through preferential pathways, such as macropores, can bypass mineral soil layers where sorption and microbial processing would otherwise reduce DOC, allowing DOC-rich water to reach streams quickly (Rennermalm et al., 2010). The activation of pathways is highly seasonal, with summer rainfall and wet soil

conditions causing sudden pulses of DOC (Blaurock et al., 2022; Stewart et al., 2024). Consistent with this, Tiwari et al. (2014) found that in the Krycklan catchment, deep groundwater inputs and subsurface flow-path connectivity strongly influence DOC concentrations, particularly during baseflow conditions, emphasizing the need to account for groundwater dynamics in catchment-scale DOC modeling. The absence of these pathways explains why high-flow DOC peaks are underestimated, despite baseflow DOC being reasonably captured.

This missing lateral connection also limits the model's ability to simulate the “memory effect,” where DOC accumulates in organic-rich soils during low-flow periods and is subsequently mobilized during groundwater rise or storm events (Haei et al., 2010; Yurova et al., 2008). Although streamflow helps capture some DOC export dynamics, the lack of lateral groundwater flow representation constrains the model's ability to simulate the seasonal “source shifting” and spatial heterogeneity of DOC pathways. Addressing these limitations will require implementing a groundwater routing module that enables lateral flow between SLC classes—something not yet available in the current Krycklan-HYPE framework.

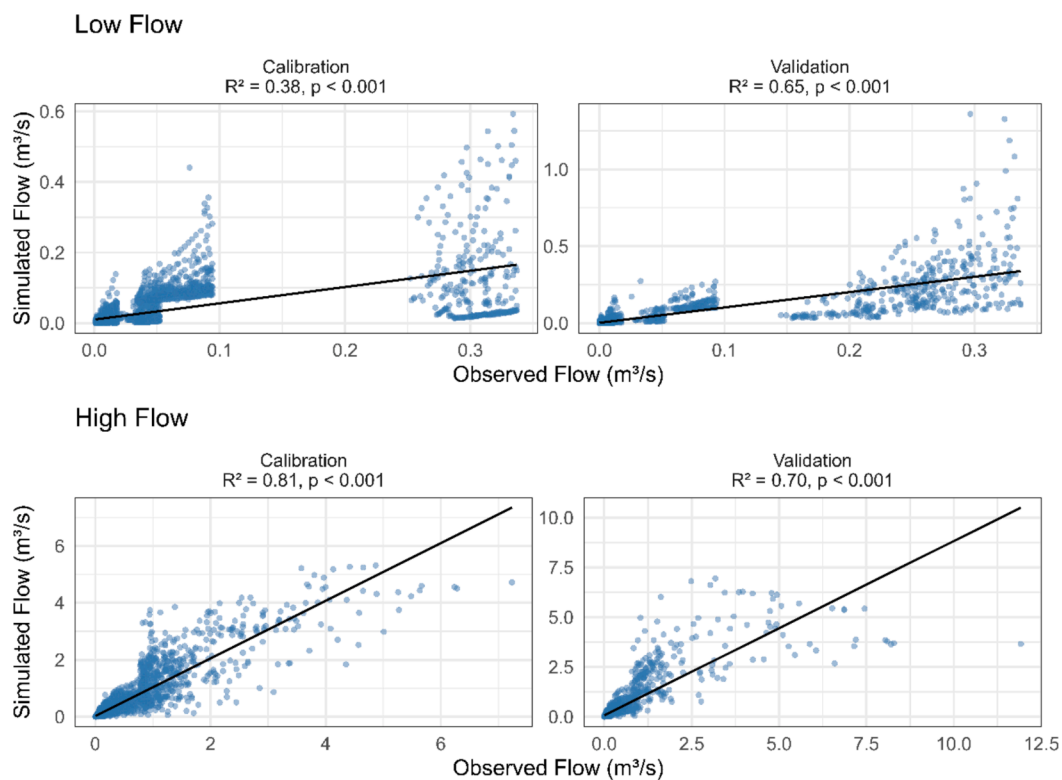


Fig. 7. Krycklan-HYPE's performance on streamflow during low flows and high flows.

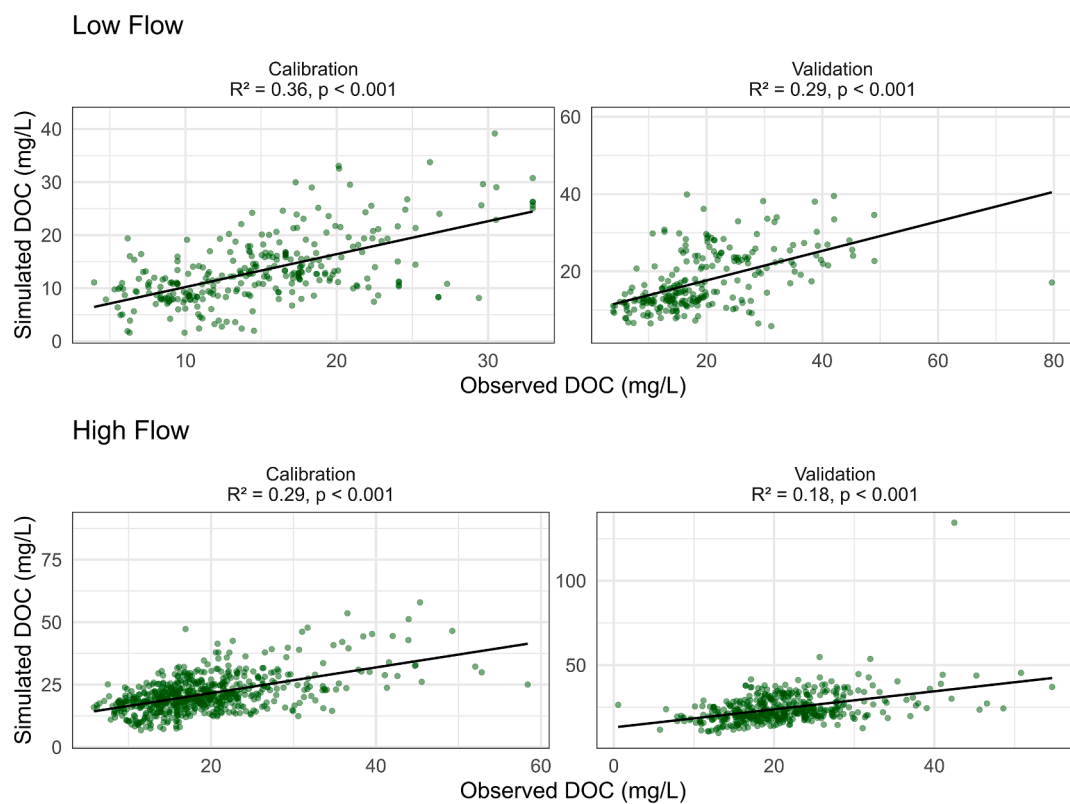


Fig. 8. The model's performance on DOC during low streamflow and high streamflow periods.

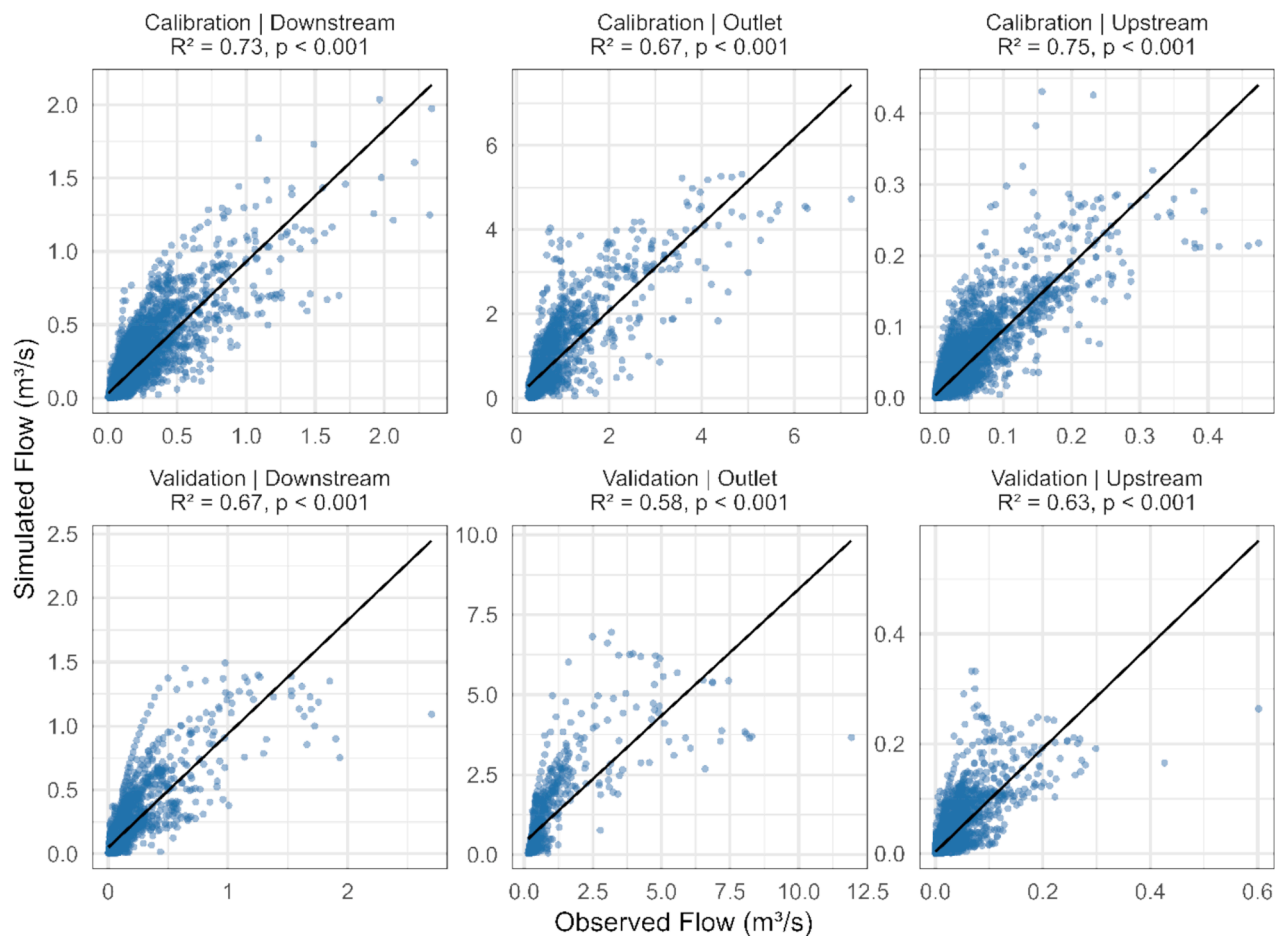


Fig. 9. Krycklan-HYPE's performance on streamflow classified by sub-catchment spatial location.

4.4. Spatial analysis of model performance

Spatial analysis also illustrated the model limitations across Krycklan (Figs. 9 and 10). Performance metrics were evaluated for upstream (C01, C02, C04, C05, C06, C07, C09, C10), downstream (C12, C13, C14, C15), and the outlet sub-catchments (C16). DOC simulation was strongest in relatively isolated sub-catchments with minimal upstream influence, such as C15 (one upstream sub-catchment), and weakest in complex downstream sub-catchments like C13 (seven upstream sub-catchments) (Appendix 1). This decline in performance is primarily attributed to the cumulative propagation of uncertainties from multiple upstream sub-catchments. As errors compound through the stream network, model predictions in downstream areas become increasingly unreliable.

This spatial performance gradient reflects the intrinsic challenges of modelling nested catchments, where upstream conditions exert a substantial influence on downstream dynamics. Hydrological connectivity plays a critical role, referring to the way that physical and chemical processes in upstream areas cascade through the catchment, ultimately shaping downstream responses (Laudon et al., 2016). In smaller, homogeneous sub-catchments, local hydrological processes predominantly control DOC variability, whereas in larger and more heterogeneous systems, DOC dynamics are influenced by the interplay between multiple upstream sources and the landscape (Laudon et al., 2011).

Another limitation concerns the Krycklan-HYPE model's inadequate representation of spatial heterogeneity in land use, soil type, and riparian zone function. Although these landscape characteristics are known to strongly influence DOC concentrations, particularly during high-flow events when connectivity to organic-rich zones increases

(Laudon et al., 2011; Tiwari et al., 2014), the current model configuration uses generalized parameterizations that do not differentiate some DOC processes among land types. For instance, it applies a uniform function to all riparian zones, ignoring differences in their DOC contribution. Grabs et al. (2012) emphasized that in organic-rich riparian zones with peat soils and shallow, fluctuating water tables act as biogeochemical hotspots, controlling much of the temporal variation in DOC export. This simplification limits the model's ability to simulate DOC dynamics accurately in mixed landscapes where spatial patterns in soil and hydrology play critical roles. Thus, improvements of the model's mechanisms to explicitly account for spatial interdependencies and feedbacks within nested catchments is needed.

4.5. Sources of model uncertainty

A deeper evaluation of the uncertainty analysis reveals that several sources contribute to the contrasting levels of confidence in streamflow and DOC simulations. Input uncertainty is an important factor, particularly for DOC, where measurement uncertainty is substantial because observations are collected at relatively low frequency. This means that short-lived DOC peaks, especially those generated during summer storms, are often missed, which weakens the calibration of DOC-related parameters and increases prediction uncertainty. Parameter uncertainty also plays a significant role. Streamflow parameters are generally well constrained, as reflected by high P-factors and low R-factors. In contrast, DOC parameters display high equifinality, with many parameter combinations yielding similar performance. This arises partly from sparse observations and strong spatial heterogeneity within the catchment,

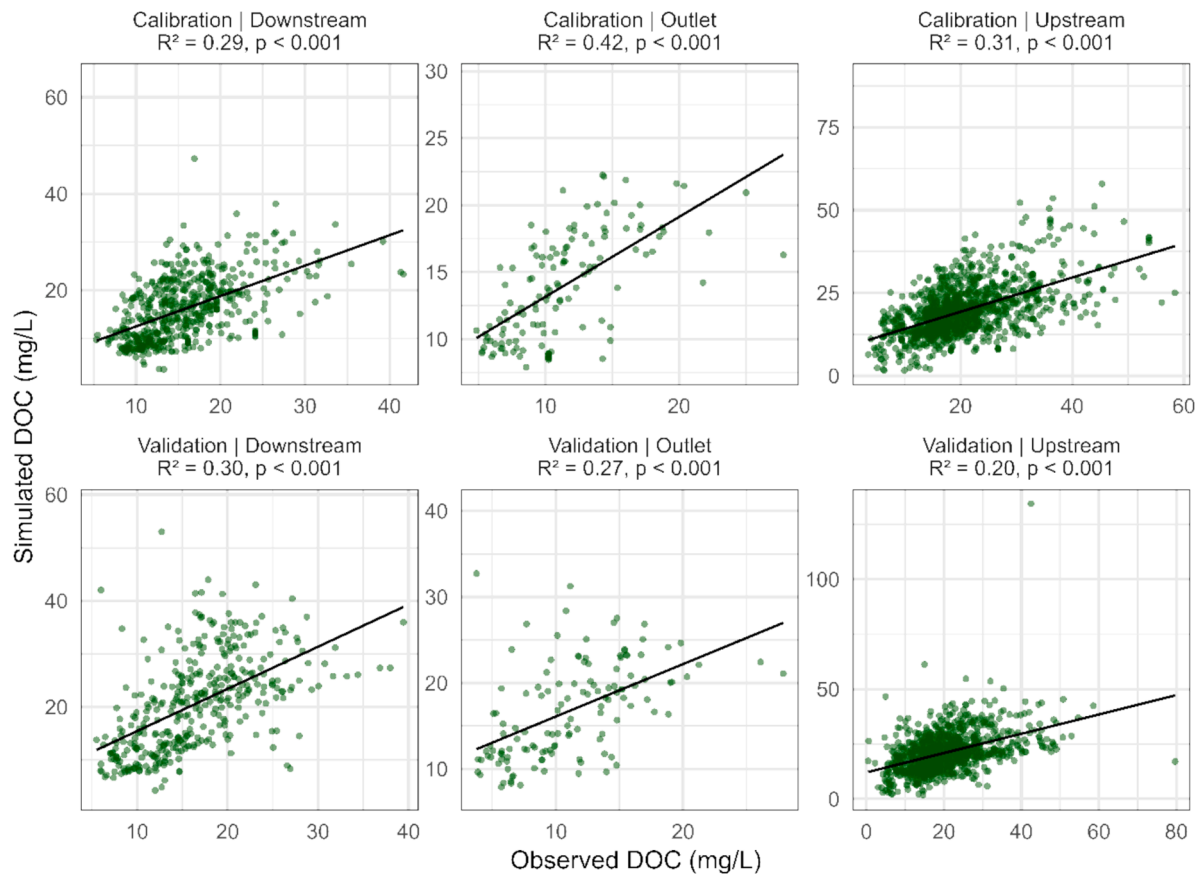


Fig. 10. Krycklan-HYPE's performance on DOC concentration classified by sub-catchment spatial location.

which limit the ability to uniquely identify key DOC parameters. As a result, wider uncertainty intervals are needed to encompass observed DOC dynamics.

The largest source of uncertainty, however, originates from model structure. Krycklan-HYPE does not explicitly simulate sorption and desorption, mineral–organic interactions, or temperature-driven microbial DOC production, even though these processes strongly influence DOC availability during warm and wet summer periods. The absence of lateral groundwater pathways further constrains the model's ability to reproduce rapid DOC flushing under high-flow conditions. These structural limitations help explain why DOC uncertainty is greatest during periods when hydrological connectivity changes rapidly, such as during summer storms, snowmelt transitions, and groundwater rise events. Finally, spatial uncertainty accumulates downstream. Errors originating in upstream sub-catchments propagate through the drainage network and amplify prediction uncertainty in larger nested sub-catchments such as C13 and C16. This compounding effect is consistent with the observed spatial gradient in DOC performance, where upstream sites with simpler hydrological structure show narrower uncertainty bounds.

5. Limitations and future work

Despite the strong performance of Krycklan-HYPE in simulating streamflow, several limitations emerged in its representation of DOC dynamics, as discussed above. Many catchment-scale DOC models incorporate processes that are currently simplified or absent in Krycklan-HYPE. For example, the SEIMS model simulates sorption, desorption, and microbial activities in wetlands by dividing DOC into different functional portions (Liu et al., 2024). In Krycklan-HYPE,

microbial mineralization is represented only implicitly, similar to in the INCA-C model. A more explicit representation could account for key controls such as soil temperature and moisture. In SWAT-Carbon, DOC recharge to the shallow aquifer is calculated using an exponential decay function, with DOC subsequently transported to deeper aquifers and eventually to the main stream (Du et al., 2019).

Future work should therefore focus on addressing these limitations by (i) incorporating explicit sorption and mineral interaction modules, (ii) improving groundwater–riparian–stream connectivity representations, (iii) developing spatially differentiated parameterizations that reflect land-use and soil heterogeneity in DOC module, and (iv) exploring data assimilation techniques to better constrain DOC dynamics during periods of rapid hydrological change. These developments could be achieved by directly extending the existing model formulations. For example, Eqs. (7) and (8), which describe the temporary DOC pool in soils, could be augmented with additional state variables or parameters to represent sorption–desorption processes and their sensitivity to soil temperature. Similarly, Eqs. (9) and (11), which govern riparian contributions and groundwater dependency, could be reformulated to allow more dynamic groundwater storage and exchange, including lateral subsurface flow, rather than relying on fixed or lumped parameterizations. Leveraging high-resolution spatial datasets (e.g., LiDAR-based soil moisture maps, detailed vegetation indices, or isotopic tracers) may improve model input and support more accurate simulations (Bajracharya et al., 2023; Stadnyk & Holmes, 2023). Enhanced monitoring with higher-frequency DOC measurements would also improve model calibration and validation. Together, these advances could substantially improve our ability to simulate terrestrial–aquatic carbon linkages in boreal catchments. Finally, hybrid modeling approaches that combine physically-based models with data-driven

techniques (e.g., machine learning) may offer a promising avenue to capture the nonlinearities and scale dependencies inherent in DOC transport.

6. Conclusions

This study introduced the Krycklan-HYPE model and provided a comprehensive evaluation of its ability to simulate streamflow and DOC across the Krycklan catchment; a heterogeneous boreal landscape characterized by complex hydrological connectivity. Results demonstrated that the model consistently reproduced streamflow at multiple spatial scales, with good calibration and validation performance supported by narrow uncertainty bounds. The model was able to simulate DOC dynamics but with lower accuracy, reflecting structural model limitations, data constraints, and the intrinsic complexity of DOC processes, particularly during high flows and in downstream sub-catchments affected by accumulated upstream uncertainty, as well as the sources shifting during winters. This highlights the need to incorporate key missing processes such as sorption, lateral groundwater flow, and riparian connectivity. Moreover, the observed trade-off between streamflow and DOC performance suggests that current model structure may inadequately integrate the hydrological and biogeochemical drivers of DOC export. Spatial analysis further showed declining performance in downstream catchments due to cumulative uncertainties and oversimplified representation of upstream–downstream coupling and distributed process. These findings emphasize that Krycklan-HYPE demonstrates the potential of process-based models to simulate carbon cycling across nested catchments, and provides a reliable hydrological foundation but requires structural refinements to improve DOC representation. By incorporating missing processes and enhancing spatial differentiation, the model could provide more accurate predictions of DOC export and better inform management of aquatic carbon fluxes under changing environmental conditions.

CRediT authorship contribution statement

Renkui Guo: Writing – review & editing, Writing – original draft,

Appendix

Appendix 1. The model performance for streamflow and DOC simulations for all sub-catchments in Krycklan. This table summarizes the model performance for each subcatchment. The calibration period is 2011–2015, and the validation period is 2016–2020. The performance metric used is KGE, calculated from the best-performing parameter set. The temporal resolution is daily.

Sub-catchments	Calibration		Validation	
	Streamflow	DOC	Streamflow	DOC
C01	0.70	0.41	0.59	0.16
C02	0.55	0.25	0.43	0.10
C04	0.81	0.31	0.83	0.17
C05	0.72	0.26	0.48	0.23
C06	0.64	0.51	0.62	0.37
C07	0.69	0.47	0.53	0.12
C09	0.70	0.50	0.50	0.36
C10	0.82	0.44	0.52	0.33
C12	0.80	0.47	0.61	0.21
C13	0.79	0.11	0.71	−0.10
C14	0.50	0.38	0.41	0.06
C15	0.79	0.59	0.58	0.58
C16	0.68	0.57	0.65	0.27
C20	0.72	0.43	0.35	0.05

Validation, Software, Methodology, Formal analysis, Data curation, Conceptualization. **Andrea L. Popp:** Writing – review & editing, Resources, Methodology. **Martin Berggren:** Writing – review & editing, Supervision. **Junzhi Liu:** Writing – review & editing. **Jiaojiao Liu:** Writing – review & editing. **David Gustafsson:** Writing – review & editing, Resources, Methodology. **Zheng Duan:** Writing – review & editing, Supervision, Resources, Methodology, Funding acquisition, Conceptualization.

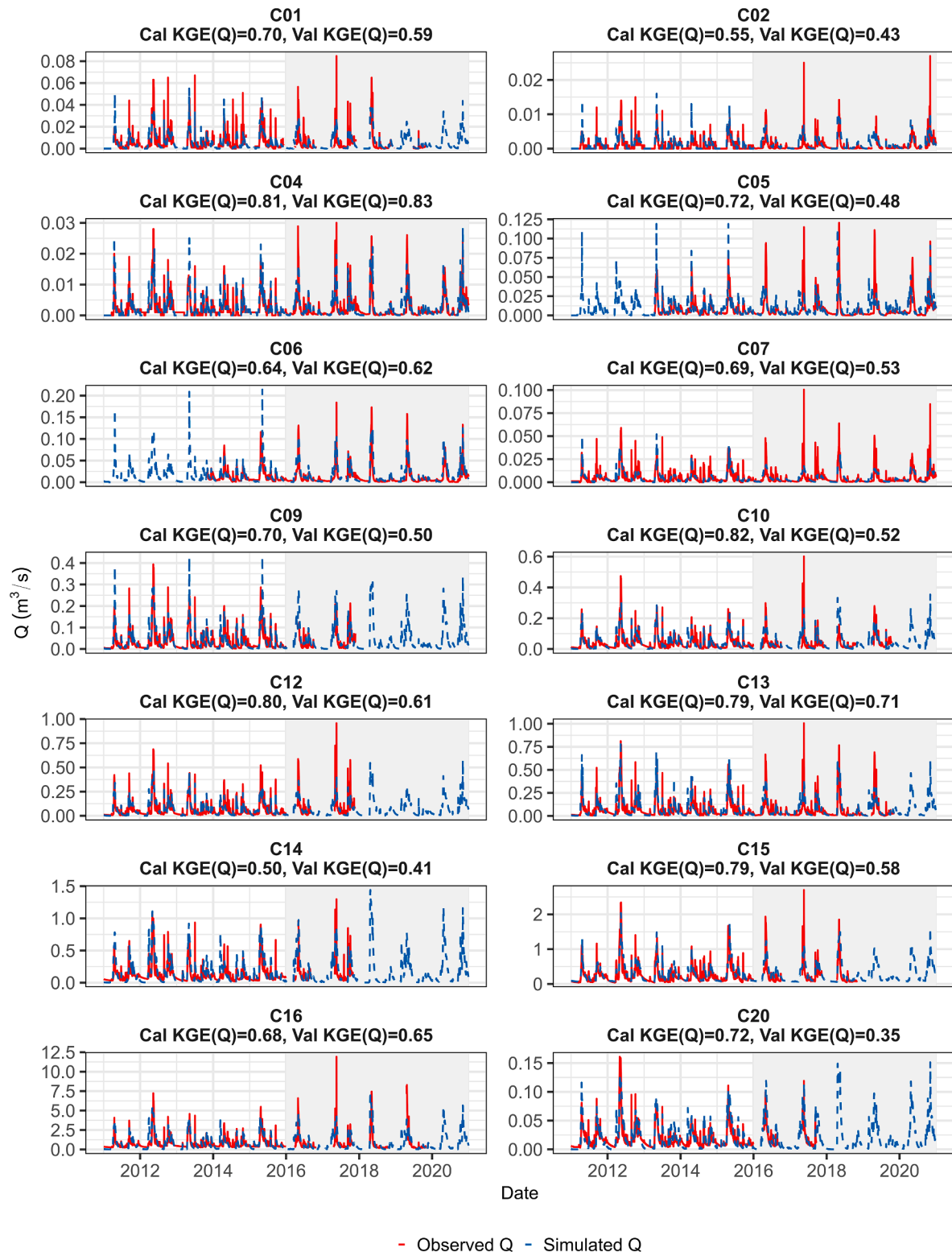
Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

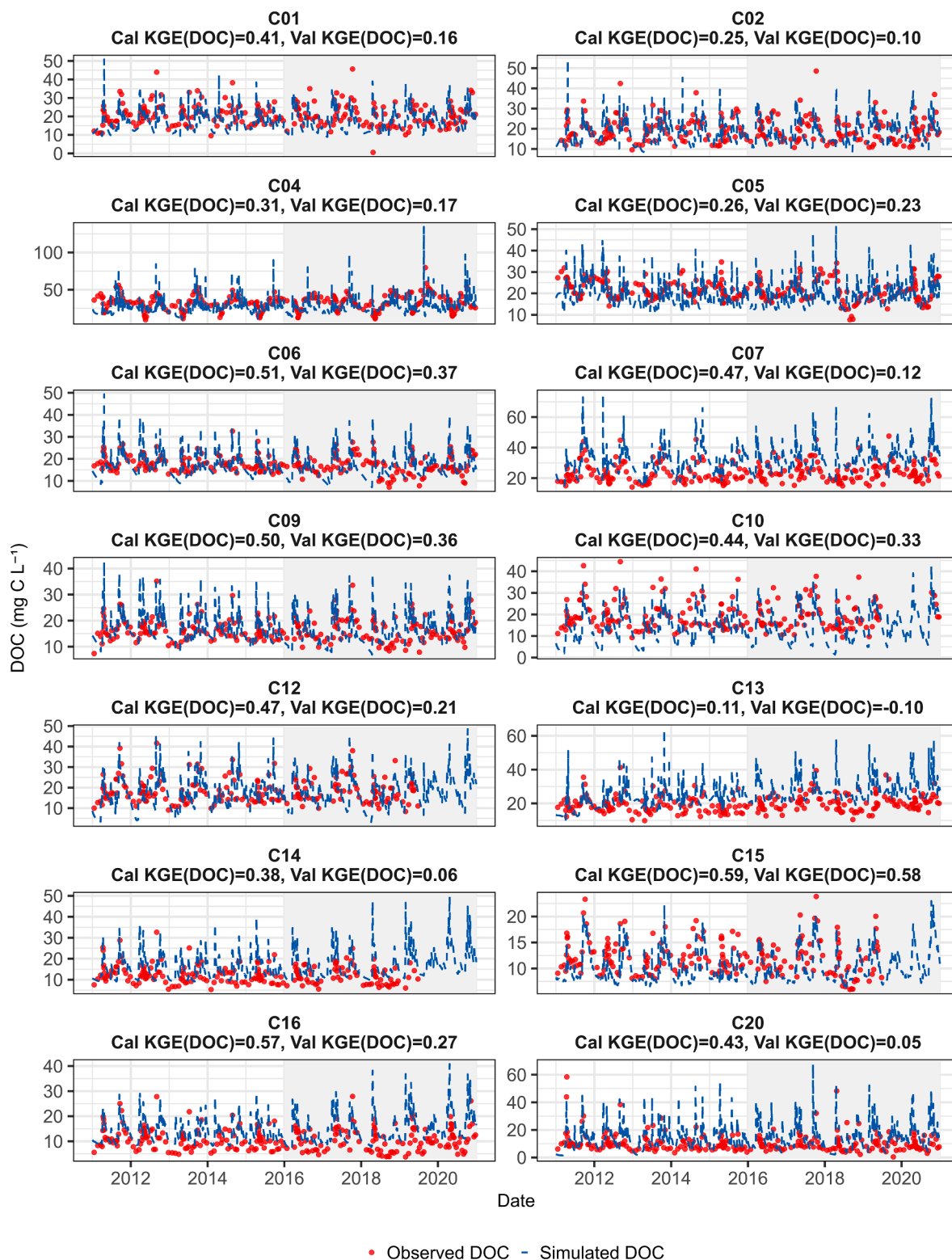
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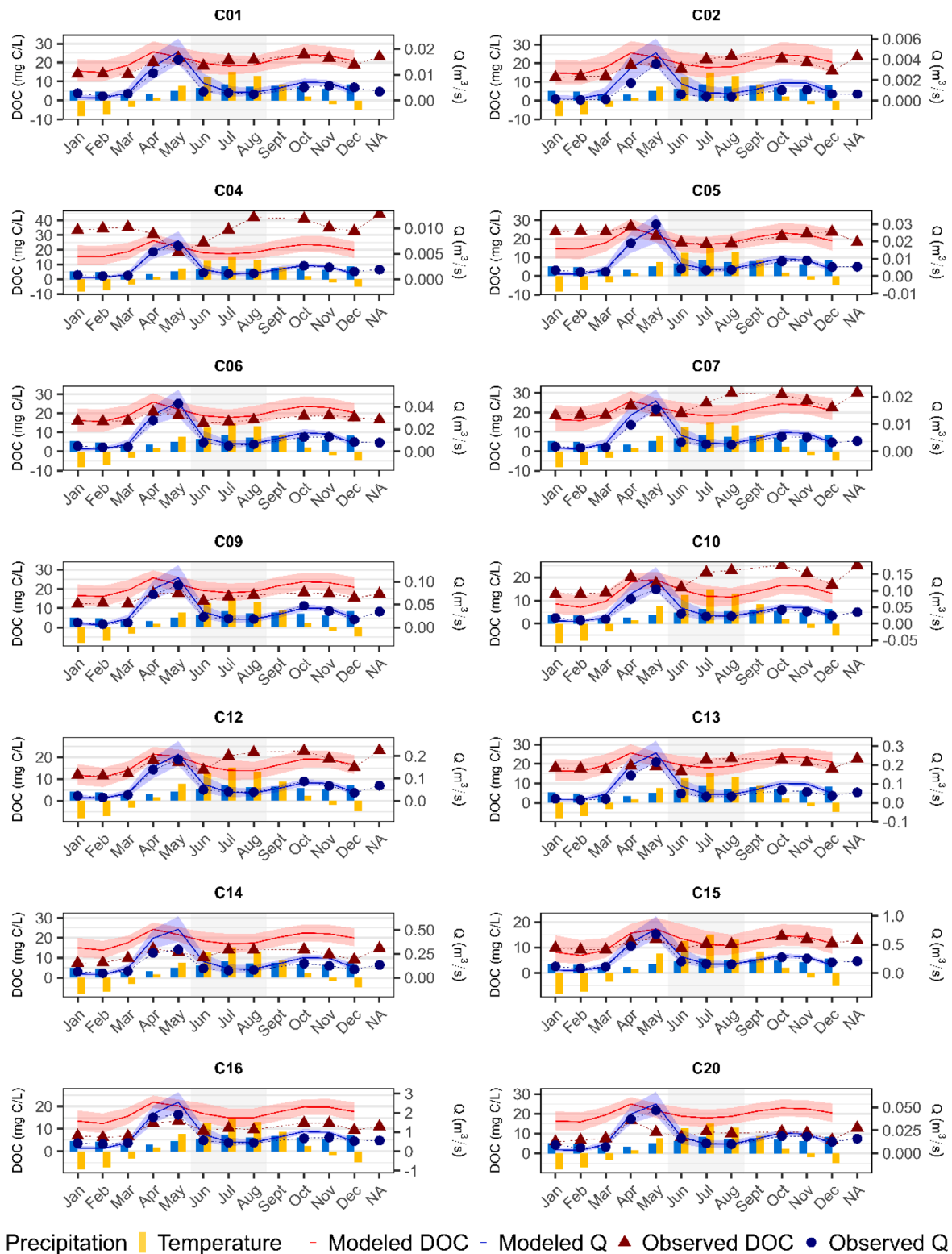
Appendix 2. Daily streamflow simulation for all sub-catchment from 2011 to 2020, calculated from the best parameter set. Cal represents calibration, Val represents validation. The calibration period is 2011–2015, and validation period is 2016–2020. The grid background indicates the calibration period and the grey shadow background indicates the validation period.



Appendix 3. Daily DOC simulation for all sub-catchment from 2011 to 2020, calculated from the best parameter set. Cal represents calibration, Val represents validation. The calibration period is 2011–2015, and validation period is 2016–2020. The grid background indicates the calibration period and the grey shadow background indicates the validation period.



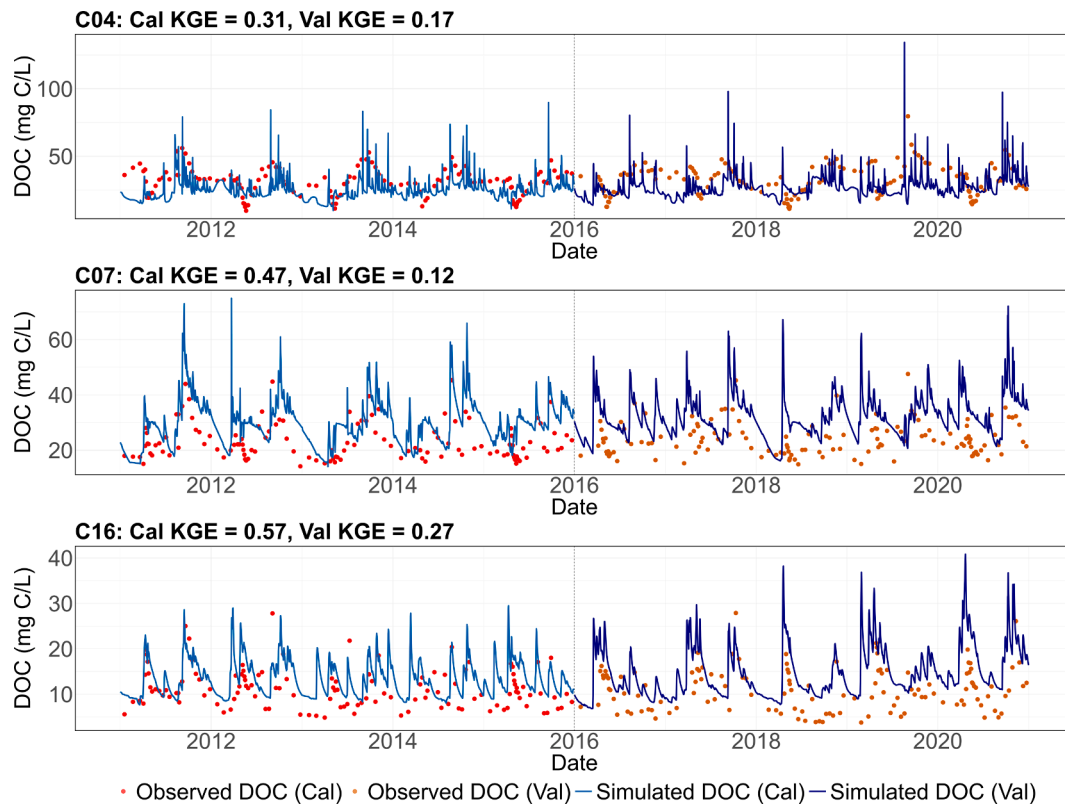
Appendix 4. Streamflow and DOC monthly dynamic in Kycklan. Monthly average temperature and precipitation during 2011–2020 are also shown. Summer months (Jun, July, August) are highlighted with grey background.



Appendix 5. 95PPU uncertainty evaluation of the model for both streamflow and DOC. The uncertainty was calculated by the top 100 best simulation among 10,000 model runs.

Sub-catchments	Calibration				Validation			
	Streamflow		DOC		Streamflow		DOC	
	P –Factor	R –Factor	P –Factor	R –Factor	P –Factor	R –Factor	P –Factor	R –Factor
C01	93.04%	2.91	93.91%	4.69	80.00%	4.57	92.31%	3.71
C02	97.52%	3.58	93.39%	4.91	87.18%	3.63	92.31%	4.79
C04	94.62%	3.23	54.62%	2.37	90.08%	3.16	59.54%	2.24
C05	92.65%	3.21	100.00%	6.59	85.25%	2.61	96.72%	5.11
C06	96.08%	3.23	98.04%	6.57	89.34%	2.85	84.43%	5.53
C07	95.42%	3.43	86.26%	3.62	91.54%	3.28	90.77%	4.13
C09	87.02%	2.85	90.08%	5.62	93.10%	4.72	79.31%	4.32
C10	91.54%	3.16	76.92%	2.99	96.97%	5.24	83.33%	3.55
C12	90.08%	2.98	83.21%	3.38	96.88%	3.56	84.38%	3.49
C13	93.13%	3.42	92.37%	4.64	91.30%	3.36	91.30%	4.20
C14	97.71%	4.65	75.57%	4.75	96.77%	6.21	77.42%	5.28
C15	93.13%	3.23	93.89%	6.00	98.18%	4.13	98.18%	4.71
C16	94.66%	3.93	70.23%	4.41	93.42%	3.40	65.79%	3.72
C20	95.38%	3.39	40.77%	2.80	100.00%	4.99	29.63%	4.91

Appendix 6. DOC simulation with respect to wetland coverage. Including daily DOC simulation among subcatchments with different wetland fractions: C04: Wetland > 50%, C07: Wetland = 20%, C16: Wetland < 10%. The calibration period is 2011–2015 and validation period is 2016–2020.



Appendix 7. Average temperature and precipitation in different seasons in Krycklan across 2011–2020. Seasons are defined as: Winter: December–February, Spring: March–May, Summer: Jun–August, Autumn: September–November.

	Spring	Summer	Autumn	Winter
Temperature (°C)	2.0	13.6	3.0	−6.7
Precipitation (mm/day)	1.1	2.0	1.9	1.7

Data availability

Data will be made available on request.

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