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Explicit Representation and Calibration of Different Landscape Units for a Robust Catchment DOC Export Model

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Abstract. Elevated dissolved organic carbon (DOC) concentrations are a major concern for ecosystems and drinking water supply. Data-driven studies revealed variable functioning of different landscape units (upland, riparian zone, and groundwater) in catchment DOC mobilization and export. However, lumped and landscape-explicit (separating upland and riparian zone) model structures are generally calibrated to stream DOC concentrations, while the internal DOC dynamics often do not receive sufficient attention. Here, we developed a flexible model with a lumped and landscape-explicit structure for four headwater catchments in the Harz Mountains, Germany. We evaluated these models under a baseline calibration (only using stream DOC concentration) and a constrained calibration (using stream DOC and internal DOC concentrations). Under the baseline calibration, both model structures can reasonably represent stream DOC dynamics in some catchments (Kling–Gupta efficiency of some behavioural simulations > 0.6), but with unreasonably high groundwater DOC. By contrast, the constrained calibration reduces the KGE for stream DOC concentrations but ensures a more realistic representation of internal DOC dynamics. Additionally, the landscape-explicit model structure is more robust than the lumped model structure under changing boundary conditions. Our study thus highlights the necessity of representing different landscape units explicitly in combination with constraining the calibration of DOC concentrations in these landscape units.

1 Introduction

Dissolved organic carbon (DOC) plays a crucial role in aquatic ecosystems, providing carbon and energy for microbial metabolism (Kaplan and Newbold, 2000; Mulholland, 2003). The amount of DOC in drinking water reservoirs, however, can be of concern as DOC can interact with chlorine used for drinking water disinfection and form harmful disinfection by-products (Bond et al., 2014). In surface water bodies, the main source of DOC is soil organic matter in terrestrial landscapes, i.e., allochthonous carbon (Mitrovic and Baldwin, 2016). Having a robust tool to quantify catchment DOC mobilization from its terrestrial sources to the river and to predict its response to changing boundary conditions has long been a research goal (Wei

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et al., 2024). Such tools and derived knowledge are important for water quality management, especially in headwater catchments that play a pivotal role in defining the quality of downstream water resources (Alexander et al., 2007).

Data-driven studies in headwater catchments have shown that the amount of DOC exported from different landscape units (the upland and riparian zone) to the stream is disproportionate to their area fractions within a catchment (Bishop et al., 2004; Blaurock et al., 2022; Dosskey and Bertsch, 1994; Ledesma et al., 2015; McGlynn and McDonnell, 2003). Often, the riparian zone is much smaller in area than the upland, but acts as the main source of stream DOC (Musolff et al., 2018; Strohmeier et al., 2013). Riparian zones in temperate and boreal systems are typically wet with shallow groundwater levels, rich in organic matter, enhancing lateral hydrological connectivity between the DOC source zone and the stream network (Ledesma et al., 2018a). The minor contribution of the upland DOC to stream DOC is argued to be due to a lack of direct hydrological connectivity between the organic layers of the upland soils and the stream. In the upland, DOC is transported vertically from the organic-rich upper soil layers into the deeper mineral subsoil and quickly gets adsorbed to the mineral phase, resulting in low DOC concentrations in the percolating water that recharges the groundwater (Kothawala et al., 2012; Ledesma et al., 2018a; Sierra et al., 2013). Therefore, the groundwater that flows into the riparian zone is low in DOC. In consequence, not all soil organic matter in a catchment is relevant for the exported DOC, but rather the fraction that can be hydrologically connected via short lateral flow paths (Zarnetske et al., 2018; Ebeling et al., 2021).

Although data-driven studies highlighted these distinct roles of the upland and riparian zones in shaping stream DOC concentrations and their dynamics, DOC modelling approaches often do not explicitly distinguish the upland and riparian zones in model structures. For example, hillslope (or lumped) model conceptualizations often consider a catchment as a single landscape unit (no separation between the upland and riparian zone) with two or more vertical layers representing the upper soil and lower soil or groundwater (Birkel et al., 2017; Grieve, 1991; Michalzik et al., 2003). Established semi- and fully-distributed water quality models such as the Soil and Water Assessment Tool model for Carbon (SWAT-Carbon; Arnold et al., 1998; Mukundan et al., 2023), the Hydrological Predictions for the Environment model (HYPE; Pers et al., 2016), the Integrated Catchments model for Carbon (INCA-C; Futter et al., 2007) exhibit detailed descriptions of how DOC is formed from soil organic matter and interacts with external inputs from plants under given temperature and soil moisture conditions. The SWAT and INCA-C models, however, do not represent the upland or riparian compartments explicitly; instead, the catchments are represented by discrete, hydrologically disconnected units (e.g., grid cells or hydrological response units - HRUs). The HYPE model has an option to represent the riparian zone (primarily designed for forest land) as an infinite DOC source to increase DOC concentrations from soil runoff before entering the stream (SMHI, 2024). However, none of the above models combine explicit landscape units with the representation of DOC processes within those landscape units.

In contrast to the aforementioned models, several others allow an explicit representation of upland and riparian zones, e.g., the modified version of the Lund-Potsdam-Jena dynamic global vegetation model and General Ecosystem Simulator (LPJ-GUESS, Tang et al., 2018; Smith et al., 2001), the ECOsystem 3D (ECO3D, Liao et al., 2019), and the DOC model developed by Birkel et al. (2014). The LPJ-GUESS and ECO3D are fully distributed and grid-based models that allow detailed representation of hydrological and DOC processing and flow routing among grid cells. These models, however, require high

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computational resources and are challenging to parameterize as well as to evaluate (Birkel et al., 2014; Tang et al., 2018; Liu et al., 2024). The simpler model developed by Birkel et al. (2014) allows the discretization of catchments into the upland, riparian, and groundwater compartments in a semi-distributed (not gridded) manner (hereinafter, we refer to this type of model as a landscape-explicit model structure). However, in contrast to LPJ-GUESS and ECO3D, this model strongly simplifies soil DOC formation and does not allow for closing carbon mass balances.

The existence of multiple model structures (Wei et al., 2024) for simulating stream DOC concentrations regardless of whether these models separate different landscape units raises the questions: (1) are lumped and landscape-explicit model structures both able to give the right results (i.e., acceptable simulations of stream DOC concentrations at the catchment outlet) for the right reasons (i.e., reasonable simulations of internal DOC concentrations) (Kirchner, 2006) when they are calibrated using stream DOC concentration only? and (2) what is the value of a constrained calibration in which information on DOC concentrations of different landscape units is used in addition to stream DOC concentrations for improving the model's credibility and physical soundness? Several studies (e.g., Bouaziz et al., 2021; Wu et al., 2023; Borriero et al., 2024) demonstrated that calibrating the model using only the integrated signal at the catchment outlet does not guarantee plausible internal modelled results. These studies call for the utilization of additional data, such as soil moisture or stable water isotope observations, to constrain the model and avoid implausibility or inconsistency. However, while the value of additional data has been demonstrated for models focusing on water quantity, applications for water quality models have been rare. Sarrazin et al. (2022) showed the value of additional "soft" data in reducing equifinality in the parameterization of a water quality model focused on catchment nitrogen transport and fate. To the best of our knowledge, the two aforementioned research questions remain unanswered in the context of DOC modelling.

The objective of this study is, therefore, to address the two aforementioned research questions on the internal consistency and value of additional data for catchment DOC models. For that, we developed lumped and landscape-explicit DOC structures in a modular DOC model, combining the strengths (model structure and DOC processes representation) of two existing models (Birkel et al., 2014; Futter et al., 2007). We then applied the proposed models in four intensively studied catchments in the Harz Mountains, Germany, to evaluate whether they produced reasonable internal DOC concentrations. We evaluated the simulated internal DOC concentration from the two model structures under a baseline calibration (using stream DOC concentration only) and a constrained calibration (using stream DOC concentration and internal DOC concentration). Furthermore, we conducted simulations using a hypothetical scenario with the two model structures (lumped versus landscape-explicit) to evaluate their credibility under changing boundary conditions. Ultimately, our study aims to provide insights into model selection, calibration, evaluation, and application for water quality management.

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2 Methodology

2.1 DOC Modelling approach

The DOC model (Fig. 1) proposed in this study is part of the water quality model (mQM) family at the Helmholtz Centre for Environmental Research - UFZ. Our model is suited to work at the catchment scale and daily time step. The DOC model we developed in this work has a flexible model structure, which can be switched between a lumped and a landscape-explicit model structure. The lumped model structure considers a combined upland and riparian zone as a single compartment plus an additional groundwater compartment (Fig. 1a), and the landscape-explicit model structure considers upland, riparian, and groundwater compartments separately (Fig. 1b). The groundwater compartment in the lumped model structure receives vertical inputs from the hillslope, which combines both upland and riparian zone into a single unit. By contrast, in the landscape explicit model structure, the groundwater compartment receives inputs only from the upland. The groundwater compartment in both model structures represents the deeper layer of water flow and solute transport to the stream below the active soil layer. Both model structures are accessed through a single executable file, and users can select which one to use in the configuration file. The lumped and landscape-explicit model structures are similar to those developed by Birkel et al. (2017) and Birkel et al. (2014), respectively. Hydrological fluxes and changes in storage are derived from the mesoscale Hydrologic Model (mHM; Kumar et al. 2013; Samaniego et al. 2010). We adapt the water fluxes and storage from mHM to represent the different landscape units in line with our DOC model structure. Specifically, we estimate the aggregated water fluxes/storages for the upland and riparian zone according to the areal fractions within a catchment (Text S1). In contrast to Birkel et al. (2014), groundwater in our landscape-explicit model structure can flow (a) directly to the stream, reflecting regional, deep groundwater flow, and (b) via a riparian zone, reflecting local, shallow groundwater flow (Laudon and Sponseller, 2018; Tóth, 1963).

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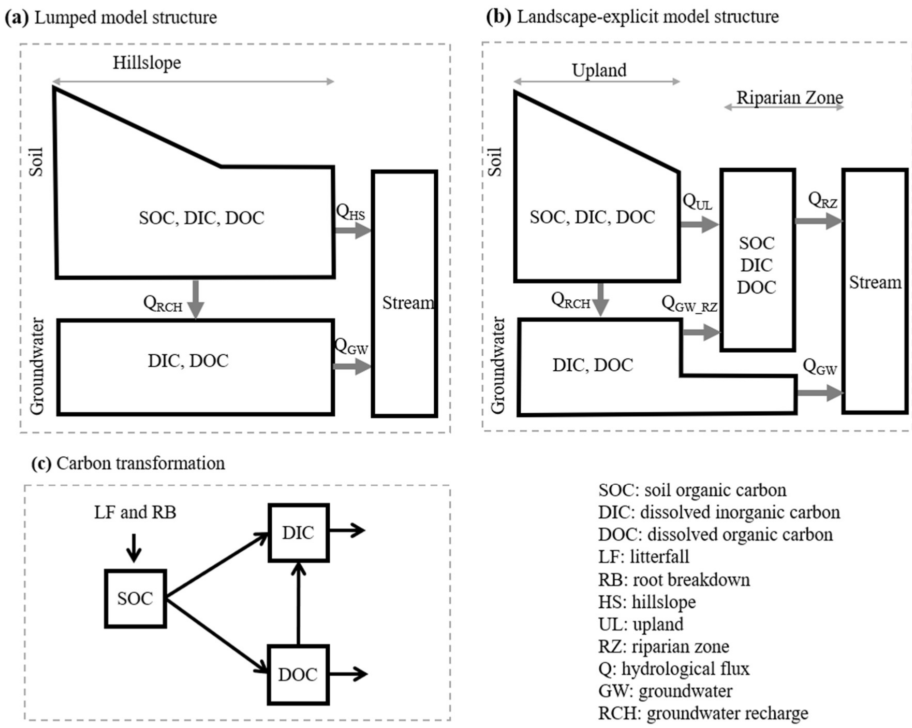

Figure 1: Conceptual representation of (a) the lumped model structure, (b) the landscape-explicit model structure, and (c) the carbon transformation among different carbon pools.

Representation of the C transformation processes in both model structures is based on the INCA-C model (Futter et al., 2007) that considers three C pools (immobile pool: soil organic carbon – SOC; mobile pools: dissolved inorganic carbon – DIC, and DOC) in the hillslope, upland, and riparian zone (Fig. 1). The transformation rates between C pools depend on soil temperature and soil moisture:

$$k_{x\rightarrow y,z}(t) = k^0_{x\rightarrow y,z} \cdot \eta^{(T_{soil}(t) - \theta)/10.0}, \quad (1)$$

$$k_{x\rightarrow y,z}(t) = k^0_{x\rightarrow y,z} \cdot \frac{(SMD_{max} - SMD(t))}{SMD_{max}}, \quad (2)$$

where k^0 (-) is the base rate, the subscripts x and y indicate the type of C pool (SOC, DIC, or DOC), z indicates upland (UL) or riparian zone (RZ) in the landscape-explicit model structure, or the hillslope (HS) in the lumped model structure (e.g., $k^0_{SOC\rightarrow DOC,UL}$(day^{-1}) is the base transformation rate from SOC to DOC in the upland), t (day) is time, η (-) is the soil temperature multiplier, θ (°C) is the base temperature offset, SMD (mm) is soil moisture deficit depending on the field capacity (FC) and current soil moisture, SMD_{max} is the maximum SMD – the driest condition (calibrated threshold value) at which transformation

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between different carbon pools can take place, and T_{soil} (t) (°C) is soil temperature. Soil temperature at day t is calculated based on the mean antecedent air temperature on the previous n days, as follows:

$$T_{soil}(t) = \frac{\sum_{i=t-n}^{t} T_{air}(i)}{n+1}, \tag{3}$$

where T_{air} (i) (°C) is the daily mean air temperature at day i (i = t-n, t), and n is the model parameter. This method was demonstrated to be effective in approximating soil temperature from air temperature in the study area (Fig. S1). We represent the net transformation between SOC and DOC using an effective transformation rate ($k_{SOC\rightarrow DOC,z}(t)$) instead of representing the transformation of DOC to SOC and SOC to DOC explicitly, like the INCA-C model does. This simplification assumes a net transfer of SOC to DOC and aims to reduce equifinality.

In the groundwater compartment, we consider the two soluble C pools (DIC and DOC) and the transformation from DOC to DIC, but no SOC and no inputs from litterfall and root breakdown. The transformation rate from DOC to DIC is not constrained by soil moisture and temperature, as this is a fully saturated zone and groundwater temperature varies minimally throughout the year.

The SOC balance equations for the UL, RZ, and HS are:

$$\frac{\partial M_{SOC,z}(t)}{\partial t} = f_z \cdot \left(LF_z(t) + RB_z(t)\right) - m_{SOC\rightarrow DOC,z}(t) - m_{SOC\rightarrow DIC,z}(t), \tag{4}$$

where the subscript z indicates the upland (UL) or riparian zone (RZ) in the landscape-explicit model structure, or the hillslope (HS) in the lumped model structure, M (kg ha^{-1}) is the SOC mass in the hillslope, upland, or riparian zone, m (kg ha^{-1} day^{-1}) is the C flux transferred between different C pools, f (-) is the areal fraction of the hillslope (f_{HS}), upland (f_{UL}), or riparian zone (f_{RZ}) within a catchment (lumped model structure: f^{HS} = 1), LF and RB (kg ha^{-1} day^{-1}) are litterfall and root breakdown, respectively. LF occurs at a user-specified period of the year, and RB occurs throughout the year at a constant rate (Futter et al., 2007).

The DOC balance equations for the HS and GW of the lumped model structure are:

$$\frac{\partial M_{DOC,HS}(t)}{\partial t} = m_{SOC\rightarrow DOC,HS}(t) - m_{DOC\rightarrow DIC,HS}(t) - m_{DOC,HS\rightarrow STREAM}(t) - m_{DOC,HS\rightarrow GW}(t), \tag{5}$$

$$\frac{\partial M_{DOC,GW}(t)}{\partial t} = m_{DOC,HS\rightarrow GW}(t)(t) - m_{DOC\rightarrow DIC,GW}(t) - m_{DOC,GW\rightarrow RZ}(t) - m_{DOC,GW\rightarrow STREAM}(t), \tag{6}$$

The DOC balance equations for the UL, RZ, and GW of the landscape-explicit model structure are:

$$\frac{\partial M_{DOC,UL}(t)}{\partial t} = m_{SOC\rightarrow DOC,UL}(t) - m_{DOC\rightarrow DIC,UL}(t) - m_{DOC,UL\rightarrow RZ}(t) - m_{DOC,UL\rightarrow GW}(t), \tag{7}$$

$$\frac{\partial M_{DOC,RZ}(t)}{\partial t} = m_{SOC\rightarrow DOC,RZ}(t) + m_{DOC,UL\rightarrow RZ}(t) + m_{DOC,GW\rightarrow RZ}(t) - m_{DOC\rightarrow DIC,RZ}(t) - m_{DOC,RZ\rightarrow STREAM}(t), \tag{8}$$

$$\frac{\partial M_{DOC,GW}(t)}{\partial t} = m_{DOC,UL\rightarrow GW}(t)(t) - m_{DOC\rightarrow DIC,GW}(t) - m_{DOC,GW\rightarrow RZ}(t) - m_{DOC,GW\rightarrow STREAM}(t), \tag{9}$$

where m (kg C ha^{-1} day^{-1}) is the C flux transferred between different C pools or the mobile C flux (DOC flux) from one model compartment to another via hydrological fluxes (e.g., from the groundwater to the stream GW→STREAM, hydrological fluxes

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can be found in Text S1). In each compartment, we used a well-mixed assumption, meaning that the DOC concentration in the outflow is identical to the DOC concentration within that compartment.

The mobile C flux between different model compartments is calculated based on hydrological fluxes and the well-mixed assumption. The C flux transferred between C pools is calculated as follows:

$$m_{x\rightarrow y,z}(t) = k_{x\rightarrow y,z}(t) \cdot M_{x,z}(t), \quad (10)$$

where x could be SOC or DOC and y could be DOC, or DIC, and $k_{x\rightarrow y,z}(t)$ is calculated based on (Eqs. 1-2) while $k_{x\rightarrow y,z}(t)$ is $k^0_{x\rightarrow y,z}$ for the groundwater (z is GW).

The total DOC fluxes exported to the stream from the lumped (Eq. 11) and landscape-explicit (Eq. 12) model structures are:

$$m_{DOC,STREAM}(t) = m_{DOC,RZ\rightarrow STREAM}(t) + m_{DOC,GW\rightarrow STREAM}(t), \quad (11)$$

$$m_{DOC,STREAM}(t) = m_{DOC,UL\rightarrow STREAM}(t) + m_{DOC,GW\rightarrow STREAM}(t), \quad (12)$$

We did not include instream DOC processes within the current version of our model. In headwater catchments in temperate regions, stream DOC processing is less relevant compared to high stream order catchments (Creed et al., 2015).

2.2 Study Area and Available Data

The study area consists of four neighbouring catchments (Kalte Bode, Warme Bode, Rappbode, and Hassel) located in the Harz Mountains, Germany (Fig. 2). These catchments drain into a system of connected reservoirs, including Germany's largest drinking water reservoir, the Rappbode reservoir, serving more than one million people (Rinke et al., 2013). The four study catchments differ in terms of catchment characteristics and hydrological conditions (Table 1). The catchment areas and average elevations range from 38.4 to 98.0 km2 and 504 to 609 m above mean sea level, respectively. The annual average precipitation varies from 789 to 1177 mm, increasing with increasing average catchment elevation. All catchments are dominated by a bedrock of Palaeozoic shales overlain by cambisols on the hillslopes and gleysols in the riparian zones. The Kalte Bode is an exception with the northwestern half being dominated by granite bedrocks and leptosols (Wollschläger et al. 2017).

Spruce forests are the dominant land cover type in the Kalte Bode, Warme Bode, and Rappbode, while agricultural land is the dominant land cover type in the Hassel. However, a large fraction of the forest has died since 2018 due to a prolonged drought and subsequent bark beetle infestations (Musolff et al., 2024; Popkin, 2021). Data after 2018 were not used in this study.

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Table 1. Catchment characteristics. The annual average rainfall and streamflow were calculated for the 2010-2018 period, and the main land uses were calculated from CORINE land cover 2018.

Catchment characteristics	**Kalte Bode**	**Warme Bode**	**Rappbode**	**Hassel**
Catchment area (km^2)	51.1	97.0	39.4	42.8
Riparian area (%)	8.7	11.0	10.6	19.1
Coniferous forest area (%)	85.3	88.4	71.8	25.2
Broad-leaved and mixed forest area (%)	2.7	0.3	3.3	10.6
Pasture area (%)	6.9	6.4	18.8	37.2
Annual average rainfall (mm/year)	1177	1098	968	789
Annual average streamflow (mm/year)	622	662	395	386
Runoff ratio	0.52	0.60	0.40	0.48
Mean elevation (m.a.s.l)	679	585	543	504

The area fraction of the riparian zone in the four catchments varies from 8.7 to 19.1% (Table 1). These riparian zone areas were calculated using a threshold value of the topographic wetness index (TWI) derived from a 25 m European Digital Elevation Model (EU-DEM). Upper percentiles of the TWI were previously shown to be a robust measure of the abundance of riparian zones within catchments (Musolff et al., 2018). The TWI threshold of 6.9 was adjusted to match the areal extent of groundwater-dominated gley soils in the Rappbode catchment (Werner et al., 2019) and applied to all four catchments. This is the sum of all TWI cells larger than 6.9 in the catchments. As driven by topography, they are distributed close to the stream network, matching the location of the riparian zone.

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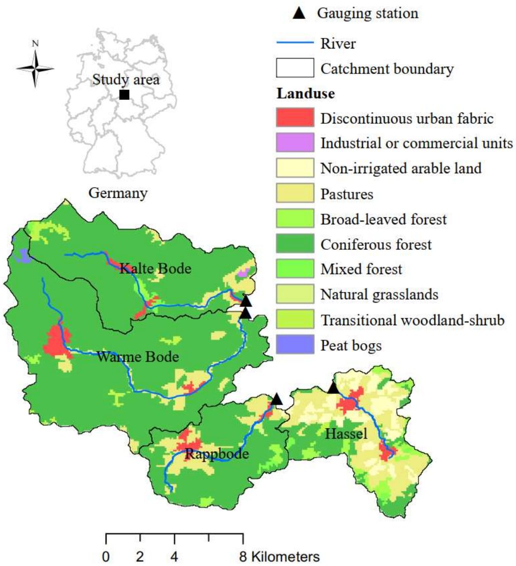

Figure 2: Location of the four study catchments in the Harz Mountains, Germany, and the CORINE land cover map in 2018.

Gridded daily meteorological data (precipitation, air temperature, and potential evapotranspiration) from 2010 to 2018 over the study area were obtained from the German Weather Service. The land cover map was taken from the CORINE land cover map in 2018. Daily streamflow from 2010 to 2018 was provided by the federal state agency responsible for hydrological monitoring in the Harz Mountains. Weekly to biweekly stream DOC concentrations from 2010 to 2018 were provided as part of the TERENO observatory (Zacharias et al., 2024) and the drinking water reservoir monitoring of inlet water quality (Kong et al., 2022).

2.3 Baseline calibration

In this study, we first calibrated the mHM (at a daily time step and 0.015625 degrees resolution) models and then the DOC models as they rely on hydrological fluxes and storages from mHM as inputs. We calibrated the mHM models using observed streamflow at the respective catchment outlets with the Dynamically Dimensioned Search (DDS) Algorithm (Tolson and Shoemaker, 2007) as it is available within the mHM framework. We used the default parameter ranges in mHM (supporting information mhm_parameter.nml). DDS starts with a random initial parameter set and then updates the parameter set iteratively within the given ranges. The updated values depend on the previous best values (according to a certain objective function) and the iteration number. After each iteration (500 in total), the probability of a parameter being updated decreases. For each basin,

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we repeated the DDS 30 times to get the respective 30 best hydrologic models (behavioural models) ranked based on the Kling–Gupta efficiency objective function value (Eq. 13) to account for parameter uncertainty.

We calibrated both models (lumped and landscape-explicit structures) using observed stream DOC concentrations at the respective catchment outlets by generating 100,000 random parameter sets using Latin Hypercube Sampling (LHS; Carnell, 2024; Stein, 1987) within selected parameter ranges based on our expert judgment and plausible values based on exploratory analyses of the model (supporting information doc_parameter.txt). This approach was used instead of DDS because it is simpler and has been demonstrated to be effective in finding behavioural parameter sets, especially when the number of parameters is small (Abbaspour, 2015). The best model (out of 100,000 runs) was selected based on the model performance (the Kling–Gupta efficiency (Eq. 13)) for stream DOC simulation. For each basin and each behavioural hydrological model, we searched for a corresponding behavioural DOC model using the aforementioned procedure. Therefore, we had 30 behavioural DOC models for each catchment.

The objective function used for calibrating the hydrological model (streamflow simulation) and DOC model (stream DOC simulation) is the Kling–Gupta efficiency - KGE (Gupta et al., 2009) expressed as follows:

$$KGE = 1 - \sqrt{(r-1)^2 + (\alpha-1)^2 + (\beta-1)^2}, \quad (13)$$

where r is the linear correlation coefficient between simulated and observed values (streamflow or stream DOC concentration), α is the ratio between the standard deviation of the simulated and the standard deviation of the observed values, and β is the ratio between the mean simulated and mean observed values. In addition, we also used other common performance metrics, namely Nash–Sutcliffe Efficiency (NSE; Nash and Sutcliffe, 1970), bias (BIAS), and R-squared (R^2) to assess the performance of the calibrated models (Text S2).

The hydrological and DOC models were calibrated for the period starting from 01/2015 to 06/2018 and validated for the period starting from 01/2010 to 12/2014. We chose this approach because the calibration period had more observation data than the validation period. The warm-up period was set to 01/2000-12/2009 because a long hydrological time series is required to avoid the effect of initial conditions (e.g., initial SOC, or DOC in different model landscape units) on simulated results.

2.4 Constrained calibration

Under the constrained calibration, we calibrated the lumped and landscape-explicit model structures using the following constraints, considering as behavioural simulation that with the highest KGE for stream DOC concentration simulation:

- The simulated average groundwater DOC concentration during the calibration period (01/2015- 06/2018) should be within the range of [0.25-2.66] mg/L. This is based on the observed groundwater DOC concentrations in six springs (median 0.5 mg/L and 90% of the values are between 0.25 and 2.66 mg/L (LHW, 2025)) within and near our study areas. In addition, observed DOC concentrations in groundwater in many other catchments worldwide are also low (median value of 1.2 mg/L with ca. 84% of the groundwater DOC samples below 5 mg/L; McDonough et al., 2020).

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- The simulated average DOC concentration in the outflows from the upland compartment during the calibration period should be less than half of that in the riparian zone ($C_{UL} < 0.5C_{RZ}$). This constraint is based on our understanding of the DOC transport processes. By that, we acknowledge that most water from the upland has undergone an infiltration into the mineral layers of the soils before laterally entering the riparian compartment. The passage through the mineral soil will significantly reduce DOC concentrations due to adsorption, as mentioned in the introduction section (Kalbitz et al., 2000; Kothawala et al., 2012; Ledesma et al., 2018a).

All other settings for the calibration were identical to the baseline calibration, including using the same initial parameter range. The first constraint (regarding groundwater concentration) was applied to both model structures (lumped and landscape-explicit). In both structures, the groundwater compartment is located below the active soil layers, and its DOC concentration is primarily shaped by mineral interactions and long residence times rather than the spatial resolution of the recharge source. Thus, we consider the groundwater compartment to be effectively equivalent in both model structures. The second constraint was applied only to the landscape-explicit structure, as the lumped model structure does not separate between the upland and the riparian zone. In addition to the aforementioned constraints, we set one additional constraint regarding the soil moisture factor in the upland of the landscape-explicit model structure. The soil moisture factor affecting C transformation in the upland should be lower than that in the riparian zone ($k_{x\rightarrow y,UL} < k_{x\rightarrow y,RZ}$; Eqs. 1-2). This constraint is based on the fact that riparian zones are wetter than upland areas given their location in the catchment in high TWI zones. Because the interaction between several model parameters that affect the soil moisture factor (e.g., field capacity, SMD_{max}, Eq. 2) can lead to unrealistic soil moisture factors, we needed to apply this constraint to account for the physical difference between the two compartments.

The technical implementation of the constrained calibration process was as follows. First, we conducted 100,000 runs using the DOC model with parameter sets generated through Latin Hypercube Sampling (LHS) as described in section 2.3, and we saved the parameter set, KGE value, average DOC concentrations in the upland, riparian zone, and groundwater, as well as the soil moisture factor in both the upland and riparian zones to reduce the model running time. Next, we applied the aforementioned constraints and selected the parameter set with the highest KGE. Finally, we reran the model with the best parameter set and extracted detailed outputs.

2.5 Scenario simulations

The scenario simulation aims to evaluate the credibility of lumped and landscape-explicit model structures calibrated with different constraints. We tested whether the lumped and landscape-explicit model structures could simulate stream DOC concentrations within a reasonable range for a hypothetical scenario where boundary conditions were changed. Specifically, we rerun the models from the baseline and constrained calibration methods with an increase of C input of 5 kg ha^{-1} day^{-1} in the upland starting in 2015 (3 years of modelling under increased inputs). The initial range for calibration is [3, 12] kg ha^{-1} day^{-1} and therefore, C input in the scenario simulation could be from 8 to 17 kg ha^{-1} day^{-1}, depending on the behavioural models found in the baseline and constrained calibration.

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Results from previous studies could provide context for evaluating the results of this exercise. For example, a previous data-driven study in one of our catchments suggests that an assumed increase in C availability following forest-dieback in the upland will not lead to a significant increase in stream DOC concentrations (Musolff et al., 2024). This can be attributed to a lack of hydrological connection of the upper upland soil layers with the stream, whereby a significant proportion of the increased C availability is processed in the upland soils and returned to the atmosphere as CO_2, while the rest of the DOC will be adsorbed in deeper mineral soil layers as the water percolates deeper into the groundwater (Musolff et al., 2024; Mikkelson et al., 2013; Kalbitz et al., 2000). Thus, we expect only minor changes in stream DOC concentrations under the scenario simulation for the model to produce credible results.

Technically, the increased C input was represented in the model as an increase in root breakdown (RB) rate. The implementation of this scenario in the landscape-explicit model structure is straightforward as we have the upland and riparian zone explicitly represented. In the lumped model structure, this amount of C input increase was weighted by the areal fraction of the upland and was applied over the whole catchment.

3 Methodology

3.1 Hydrologic simulation

Visual assessment of the results shows that the seasonality of streamflow, low in summer (June to August) and fall (September to November), high in winter (December to February) and spring (March to May), from all catchments was well captured by the models (Fig.3, Fig. S2a). Most behavioral models tend to underestimate high-flow events (Fig. 3a). The simulated average yearly hydrological fluxes show that Warme Bode, Rappbode, and Hassel have the highest outflow (as a percentage of streamflow) from the upland (or the full hillslope when referring to the lumped model structure) (median values > 80%) while that of the Kalte Bode is lower (median value ~ 60%) (Fig. S3). The average annual groundwater discharge from the groundwater compartment in the Kalte Bode (median value ~ 35%) is much higher than that of the Warme Bode, Rappbode, and Hassel (median values: ~10% to ~15%) (Fig. S3) due to the presence of granite bedrocks and leptosols, creating higher groundwater recharge and flow. In both model structures, the amount of water discharge from the groundwater compartment is the same (Fig. 1). However, in the landscape-explicit model structure, between 10% (Warme Bode) and 35% (Hassel) of the groundwater discharge flows to the riparian zone before flowing to the stream.

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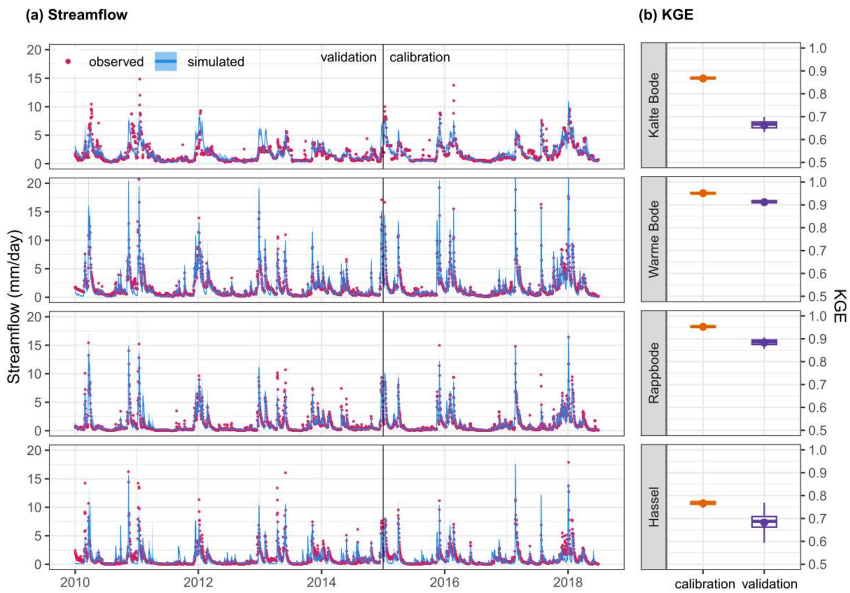

Figure 3: (a) Time series of observed and simulated streamflow and (b) the model performance (KGE) of 30 behavioural streamflow simulations (the dots in the boxplots are the means). The solid lines and shaded areas (in blue) represent the medians and simulated ranges of these 30 streamflow simulations. Simulated streamflow from lumped and landscape-explicit model structures is identical; the differences between lumped and landscape-explicit model structures are the internal hydrological fluxes (Text S1).

Across all catchments, streamflow simulation in the calibration period is generally better than in the validation period: the mean KGEs of the behavioural models for the calibration period are significantly higher (p-value < 0.05; t-test) than those of the validation period. Yet, the model performances for streamflow simulation of the Warme Bode and Rappbode are comparable (mean KGEs of both calibration and validation periods are higher than 0.91 and 0.88, respectively) while those for the Kalte Bode and Hassel are slightly lower for the respective periods (mean KGEs of the behavioural models for the calibration and validation periods are 0.87 and 0.66 (Kalte Bode) and 0.77 and 0.68 (Hassel), respectively). The model performance for streamflow simulation is acceptable considering that all behavioural models achieve KGE > 0.59 (Knoben et al., 2019). Other model performance indices, e.g., NSE, BIAS, and R^2 (Figs. S4-S6) for streamflow simulation show similar patterns to those of KGE.

3.2 DOC concentration dynamics under baseline calibration of the lumped versus landscape-explicit model structure

The simulated stream DOC concentration from the two model structures in the baseline calibration partly deviates from each other (Fig. 4a-b, upper panel). For example, in the Kalte Bode and Warme Bode, the lumped model structure yields higher simulated stream DOC concentration ranges than the landscape-explicit model structure. However, both lumped and

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landscape-explicit model structures tend to miss major high-concentration events that have been observed in the Kalte Bode and Warme Bode catchments. Here, the maximum simulated stream DOC concentrations from the lumped model structure could be as high as 32 mg/L, while those in the landscape-explicit model structure are around 10 mg/L. In Rappbode and Hassel catchments, both model structures show similar simulated stream DOC (around 2 to 10 mg/L) and seasonal dynamics (high in summer and fall, low in winter and spring), which also resemble the observed data (Figs. S2b-c).

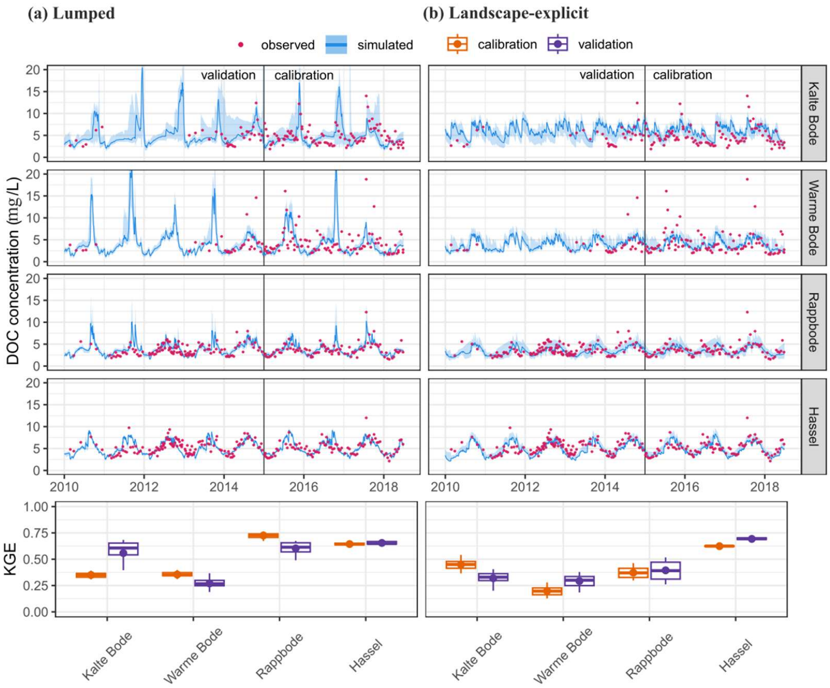

Figure 4: Time series of observed and simulated stream DOC concentrations and the model performance of 30 behavioural DOC simulations from (a) the lumped and (b) the landscape-explicit model structures during baseline calibration. The solid lines and shaded areas (in blue) represent the medians and simulated ranges of these behavioural models. The dots in the boxplots are the means.

The landscape-explicit model structure does not always have a higher model performance (higher median KGE) than the lumped model structure (Fig. 4a-b, lower panel). In the Rappbode catchment, the lumped model structure (median KGE > 0.6) outperforms the landscape-explicit model structure (median KGE < 0.5) for both calibration and validation periods. However, both model structures show a comparable model performance for the Hassel catchment with a median KGE of about 0.63. In the Kalte Bode catchment, the landscape-explicit model structure has a higher median KGE for the calibration, but a lower median KGE for the validation than the lumped model structure. The opposite is true for the Warme Bode catchment, where both model structures show the lowest median KGEs among the four catchments. We note that the ranking of the model

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performance among catchments and periods is sensitive to the performance metrics. More specifically, the NSE, BIAS, and R^2 (Figs. S4-S6) do not show the same trend across the four catchments as that of the KGE (Fig. 4).

3.3 Baseline versus constrained calibration

The simulated stream DOC concentrations with the lumped model structure under the constrained calibration are in general lower than those under the baseline calibration and observed data across all catchments (Fig. 5a - upper panel and Fig. S2b). In contrast, within the landscape-explicit model structure, there are only minor differences between the baseline and constrained calibrations at both daily (Fig. 5b - upper panel) and seasonal timescales (Fig. S2b-c). For example, in the Warme Bode during winter and spring, the interquartile ranges of the simulated stream DOC concentrations using the landscape-explicit model structure under the constrained calibration are slightly wider than those under the baseline calibration (Fig. S2c).

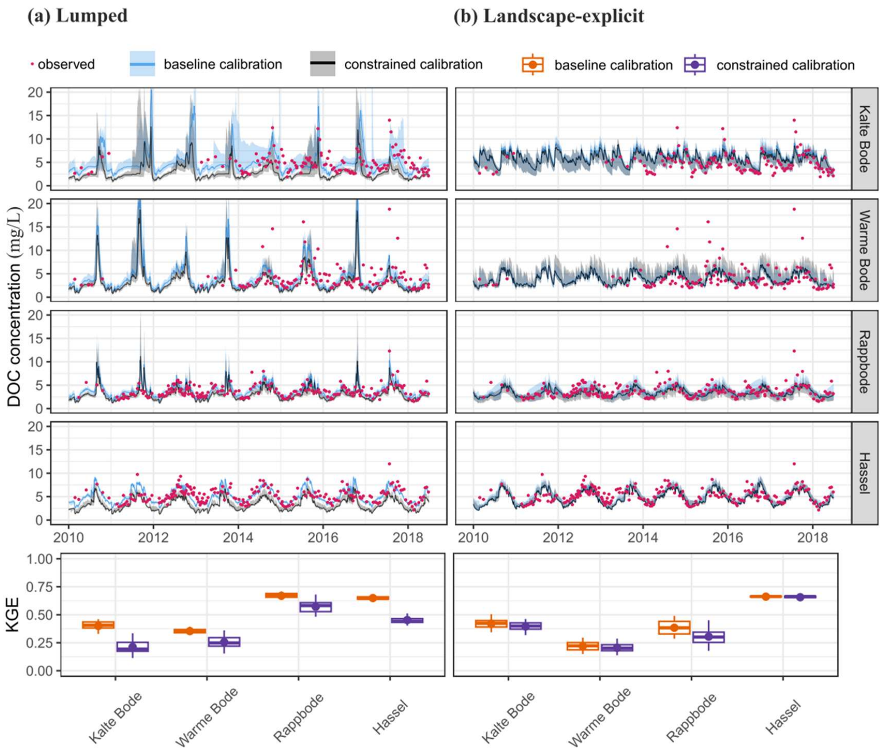

Figure 5: Observed and simulated stream DOC concentration from (a) the lumped and (b) the landscape-explicit model structures under the baseline and constrained calibrations, along with the model performance (KGE) for both calibration and validation periods together. Simulated results were taken from 30 behavioural DOC simulations. The dots in the boxplots are the means.

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With the lumped model structure and across all four catchments, the model performance (mean KGEs) for stream DOC simulation under the constrained calibration decreases significantly ($p < 0.05$) compared to that under the baseline calibration (Fig. 5a, lower panel). The magnitude of reduction in the model performance varies among catchments and models with an overall average decrease in the KGE of 0.14. In contrast to the lumped model structure, with the landscape-explicit model structure, the model performance for stream DOC simulation under the constrained calibration shows only a negligible (KGE decrease of 0.01 on average at Kalte Bode, Warme Bode, and Hassel, $p < 0.05$) or minor (KGE decrease of 0.08 on average at Rappbode, $p < 0.05$; see Fig. 5b, lower panel) decrease. The NSE and BIAS also show a decrease in the model performance under the constrained calibration with the lumped model structure across all catchments (Fig. S7). However, the R^2 values under the baseline and constrained calibration with the lumped model structure are comparable. With the landscape-explicit model structure, the NSE, BIAS, and R^2 under the constrained and baseline calibrations are comparable across all catchments (Fig. 6b).

Under the baseline calibration, most of the simulated groundwater concentrations with the lumped model structure are above the threshold level (2.66 mg/L) defined in the constrained calibration (Fig. 6a). Under the constrained calibration, the maximum simulated groundwater concentrations with the lumped model structure are slightly above 2.66 mg/L (as the constraint was imposed on the average value). Moreover, in all catchments, the simulated hillslope DOC concentrations under the constrained calibration are lower than those under the baseline calibration, especially in the Kalte Bode and Hassel (Fig. 6a). With the landscape-explicit model structure for the Kalte Bode and Warme Bode, there are minor differences in the internal DOC concentrations under the baseline and constrained calibration (Fig. 6b). In the Rappbode and Hassel catchment, however, there are clear differences in the groundwater and upland DOC concentrations under the baseline and constrained calibration (Fig. 6b). For example, the maximum simulated groundwater DOC concentrations in the Rappbode and Hassel with the landscape-explicit model structure and under the baseline calibration reach 9 mg/L while those under the constrained calibration are slightly above 2.66 mg/L. The maximum simulated upland DOC concentrations in the Rappbode and Hassel with the landscape-explicit model structure under the constrained calibration significantly decrease compared with those under the baseline calibration (e.g., Hassel: from above 15.0 mg/L to less than 5.4 mg/L).

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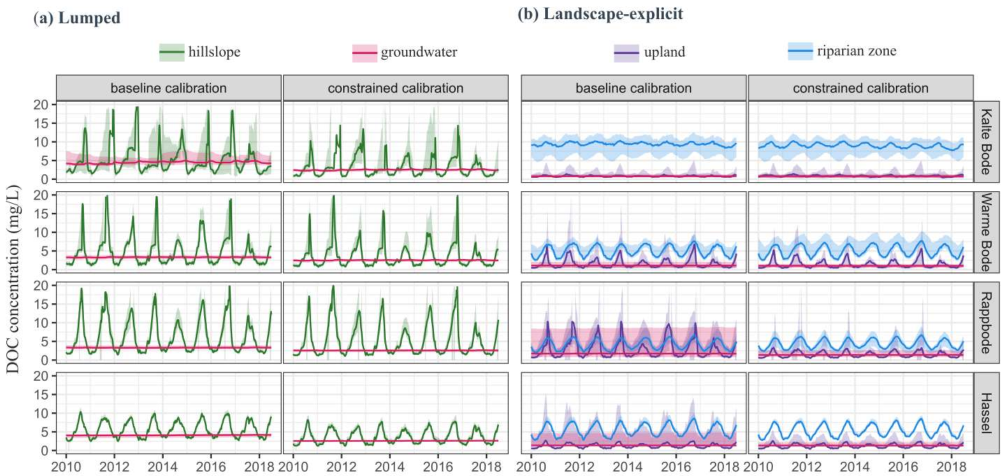

Figure 6: Internal DOC concentrations in different landscape units from (a) the lumped and (b) the landscape-explicit model structures under the baseline and constrained calibrations.

3.4 Changes in stream DOC concentrations under scenario simulations

In this section, we report results from the Hassel catchment (Fig. 7) as an example. Results obtained from the three remaining catchments (Fig. S8) are similar to those from the Hassel catchment. It is seen that with the lumped model structure (Fig. 7 – left panel), increasing C input in the upland soils will significantly increase (p-value < 0.05) stream DOC regardless of the calibration approach (mean DOC concentration increases from 5.1 to 7.0 mg/L and from 3.3 to 5.2 mg/L when using the baseline and constrained calibrated models, respectively). By contrast, using the landscape-explicit model structure (Fig. 7 - right panel), the changes in stream DOC concentration are lower than 0.1 mg/L and therefore negligible when increasing C input in both calibration approaches.

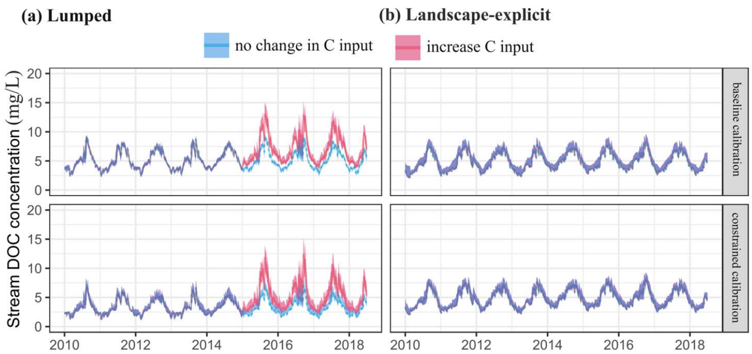

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Figure 7: Simulated stream DOC concentrations in the Hassel catchment with increasing C input by 5 kg/ha for the period 2015-2018 (a) in the hillslope of the lumped model structure, and (b) in the upland of the landscape-explicit model structure.

When increasing C input, results show that there are negligible changes (< 0.1 mg/L) in the mean groundwater DOC concentrations across all model structures and calibration methods (results were not shown here). However, there are significant ($p < 0.05$) increases in the mean hillslope DOC concentration with the lumped model structure that were calibrated under the baseline calibration (an increase of 2.7 mg/L or 45%) and the constrained calibration (an increase of 2.6 mg/L or 70%). With the landscape-explicit model structures, we found increases of 1.3 mg/L (59%) and 1.1 mg/L (83%) in the upland DOC concentrations with the models calibrated under the baseline and constrained calibrations, respectively. There are negligible changes (< 0.1 mg/L) in riparian DOC concentrations with the landscape-explicit model structures across all calibration methods.

4 Discussion

4.1 The right results for the wrong reasons? DOC dynamics under baseline calibration

Application of the lumped and landscape-explicit model structures under the baseline calibration shows that both structures can give a satisfactory model performance for stream DOC concentrations (Fig. 4). This is in line with previous studies, in which both model structures were successfully applied for stream DOC simulation (Birkel et al., 2014, 2017; Strohmenger et al., 2021). However, not all of the simulated DOC concentrations in the internal model units (e.g., hillslope, upland, and groundwater) from lumped and landscape-explicit model structures fit our process understanding and observations (section 3.3). In fact, with the lumped model structure, none of the behavioural models under the baseline calibration meets our understanding regarding low groundwater DOC concentrations. More specifically, the lumped model needs implausibly high groundwater concentrations to maintain high DOC concentrations throughout the year that cannot be generated by the variably saturated hillslope compartment. Also, with the landscape-explicit model structure, only 53% of behavioural models (across all four catchments) under the baseline calibrations meet all of our constraints (section 2.4). However, in contrast to the lumped model, the landscape-specific model structure maintains a good performance after constraining the groundwater concentrations to the observed range of DOC concentrations and the upland concentration to match our understanding of the different compartments. Examining internal DOC concentrations has often been neglected in catchment DOC models, either due to data availability or because these are not the variables of interest. Using models that inconsistently simulate internal DOC dynamics could lead to a false interpretation and potentially to wrong management decisions. Here, together with other water quality studies (i.e., Fohrer et al., 2022; Lutz et al., 2022), we emphasize the need for also evaluating concentrations and fluxes in and between internal model compartments.

Our results show that stream DOC concentration alone is not sufficient to constrain either lumped or landscape-explicit model structures in terms of internal DOC concentrations and fluxes. The interplay between different parameters affecting DOC production, together with the added complexity of having those parameters acting in different model compartments (i.e., upland, groundwater, and riparian zone) result in a myriad of model simulations that are able to reproduce stream DOC dynamics, but not necessarily able to represent landscape-internal dynamics. With more complex model structures, there is a higher degree of freedom and a higher uncertainty in model parameterization, leading to higher uncertainty in the internal DOC dynamics. For example, wider simulated groundwater DOC concentration ranges were found from the landscape-explicit model structure than from the lumped model structure in the baseline calibration (Fig. 7). This is because the amount of groundwater that flows directly to the stream in the landscape-explicit model structure is less than that in the lumped model structure (Fig. 1 and section 3.1), making the information content of observed stream DOC concentration ineffective for constraining groundwater DOC concentration. Similarly, there is also a high uncertainty in the upland DOC concentration from the baseline calibration, as DOC in the upland does not flow directly into the stream.

On the other hand, the landscape-explicit model structure enforces a conceptual understanding that also constrains, to a certain extent, the degree of freedom. More specifically, the introduction of the riparian zone compartment that upland water needs to pass, limits the instream DOC concentration range. Since the riparian zone has a constantly high soil moisture, the concentration range is mainly dictated by soil temperature (see 2.1) while contributions from upland are buffered by mixing with the riparian DOC mass. Soil moisture variations in the hillslope allow for a higher DOC concentration range that can be transferred to the stream. However, we argue that this direct connectivity does not exist in our catchments and therefore gives the right answer (peak concentrations in stream DOC are met) for the wrong reason (peak DOC comes from the dryer upland or hillslope compartment) (Musolff et al. 2021, Ledesma et al. 2018a, Ledesma et al. 2025). On the cost of implausible internal DOC fluxes, consequently, some of the catchments show a weaker model performance according to the KGE metric with the lumped compared to the landscape-explicit model structure (Warme Bode, Rappbode, Fig. 4).

Indeed, there is evidence from the Rappbode catchment that riparian zone DOC concentrations can be higher (observed up to 16 mg/L, Ledesma et al. 2025) than modelled here (range 2.5 to 9 mg/L, Fig. 6). Here, future model improvements may allow for a higher concentration range in the riparian zone by applying principles of vertical heterogeneity in water flow and DOC mobilization from riparian zones as described by Seibert et al. (2009) or Ledesma et al. (2018b).

The finding that instream DOC is not sufficient to constrain the DOC concentrations in other model compartments is supported by similar findings from previous studies, which focused on other water quality variables. Nguyen et al. (2022) found considerable uncertainty in the internal modelled results (i.e., soil nitrogen storage, groundwater nitrate concentration) when their models were only calibrated to the integrated signal (i.e., stream nitrate concentration) at the catchment outlet. They emphasized the need for more data to better constrain the model. For DOC modelling, we demonstrated that incorporating data from groundwater DOC concentrations or DOC concentrations from different landscape units (e.g., upland and riparian zones) could help to better constrain internal model states, which would otherwise be highly uncertain and likely implausible when calibrated solely based on instream DOC concentrations.

4.2 The value of a landscape-explicit structure and a constrained calibration

The results of this study demonstrate that under the constrained calibration, model performance in terms of stream DOC concentration might be compromised as a result of the applied constraints. When additional constraints are introduced, the solution space becomes more limited (Salmon-Monviola et al., 2024), potentially leading to a lower number of parameter sets able to satisfactorily reproduce stream dynamics. However, the modelled internal DOC concentrations under the constrained calibration are more consistent with our understanding and observed data (section 3.3), highlighting the value of constraining the model. The value of the landscape-explicit structure was revealed in our scenario simulations. With the lumped model structure, we could only impose the constraint on the simulated groundwater DOC concentrations, and the contribution of groundwater DOC to stream DOC is minor compared to that of the hillslope due to relatively low groundwater flow and DOC concentration (Figs. S3 and 6). Thus, the scenario in which we increased C inputs in the lumped structure led to a significant increase in simulated stream DOC concentrations, which does not match our conceptual model and our observations (Musolff et al., 2024). By contrast, with the landscape-explicit model structures calibrated under the baseline and constrained calibrations, the majority of stream DOC originates in the riparian zone. Therefore, both calibration routines show negligible changes in stream DOC concentration during the scenario simulation case, which matches our expectations based on our observations in the Rappbode catchment, where an increased C input in the upland following forest-dieback led to minor changes in the stream DOC concentrations (Musolff et al., 2024). We acknowledge that our scenario did not comprehensively represent the impacts of forest dieback, particularly concerning hydrological changes, but instead focused exclusively on an increased C input from the upland. This approach aligned with the aim of this exercise, which was to evaluate how different model structures affect simulations of stream DOC concentrations under changing boundary conditions.

4.3 Implications for model evaluation and model structure selection

The results of our study indicate that a DOC model evaluated solely on its ability to simulate stream DOC concentrations may not serve as a robust prognostic tool under changing conditions. A lumped model structure might outperform a landscape-explicit model structure for stream DOC concentration simulation (e.g., Fig. 4 - Rappbode catchment), but it is likely that the lumped model structure cannot be used for scenario exploration (section 3.4). We argue for using only model structures that can be justified (Beven and Freer, 2001). In line with the arguments presented by Beven and Freer (2001), this justification should be based on observations or qualitative understanding of the catchment processes as demonstrated in this study, even when the overall performance of the justifiable models might be lower.

With more complex models (e.g., SWAT+, INCA, HYPE), the available data may be insufficient to constrain all model parameters. Still, the models can exhibit substantial equifinality (i.e., multiple parameter sets may produce equally acceptable simulations), resulting in a wide range of potential solutions, some of which may be unrealistic. This is consistent with our own experience using a landscape-explicit model. Therefore, we recommend that modellers critically evaluate which model outputs can be used, prioritizing those that have been evaluated by direct observations or corroborated by expert knowledge.

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5 Summary and Conclusions

Elevated DOC concentrations are a major concern for ecosystems and drinking water supply from surface water reservoirs. Robust modelling tools for predicting terrestrial DOC export to the aquatic system are highly relevant. Data-driven studies revealed variable functioning of different landscape units (upland, riparian zone, and groundwater) in catchment DOC mobilization and export. Both lumped and landscape-explicit (separating upland and riparian zone) model structures are in use. They are generally calibrated to observed stream DOC concentrations, while the landscape-internal DOC dynamics often do not receive sufficient attention. Here, we developed a flexible model with a lumped and a landscape-explicit conceptualization for four headwater catchments in the Harz Mountains, Germany. We evaluated the simulated internal DOC concentrations when the model was calibrated using stream DOC concentration alone (baseline calibration) and the value of additional constraints for model calibration (constrained calibration). We further conducted scenario simulations in which we increased carbon input to the upland to evaluate the simulated response of stream DOC concentration under different model structures. The key findings from our study are listed below.

- Under the baseline calibration, both lumped and landscape-explicit model structures can reasonably represent stream DOC concentration dynamics, with none consistently outperforming the other, as performance varies across basins and evaluation metrics. However, the simulated DOC concentrations in groundwater for both model structures can be significantly higher than those from observations, indicating unrealistic internal DOC dynamics.
- The constrained calibration (accounting for physically-realistic DOC concentrations in the upland and groundwater compartments) slightly reduces model performance for stream DOC concentration simulation for the landscape-explicit model structure, but it increases the physical realism of the model in terms of internal DOC concentrations. In contrast, the performance of the lumped model structure is significantly reduced under the constrained calibration.
- For evaluating the effectiveness of spatial management on stream DOC (e.g., changes that do not occur homogeneously over the entire catchment, such as increasing C input in the upland in this study), a landscape-explicit model structure provides reasonable results, while a lumped structure does not.

While the aforementioned results might not be transferred directly to other catchments, we call for a careful evaluation of the physical realism of the DOC processes in the internal model compartments of other DOC models. This is crucial, particularly when management decisions should be robust, also under changing boundary conditions.

Code and data availability

The model source code and data used in this study can be found at https://doi.org/10.5281/zenodo.1069202 (mHM model source code), https://doi.org/10.2909/960998c1-1870-4e82-8051-6485205ebbac (CORINE land cover 2018), https://opendata.dwd.de/ (meteorological data), https://gld.lhw-sachsen-anhalt.de/ (streamflow data), https://www.ufz.de/index.php?en=48150 (UFZ forest monitor data), and https://www.eea.europa.eu/en/datahub/datahubitem-

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view/d08852bc-7b5f-4835-a776-08362e2fbf4b (EU-DEM). The mQM source code can be provided upon request from the first author.

Supplement link

The link to the supplement will be included by Copernicus, if applicable.

Author contributions

All authors contributed to the study design, including developing the conceptual DOC model, test cases, and overall manuscript structure. T.V.N. drafted the initial manuscript. A.M. and J.L.J.L. contributed to the writing and to the analysis of the results. T.V.N. developed the model code and ran all simulations.

Competing interests

Rohini Kumar is a member of the editorial board of Hydrology and Earth System Sciences.

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