*Supplement of*

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

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# Text S1. Hydrological fluxes and storages

The mHM model (Samaniego et al. 2010, Kumar et al., 2013) is a spatially explicit, grid-based model that utilizes process formulations from established models such as HBV (Bergström, 1992) and VIC-3L (Gao et al., 2009). Using a grid as the basic unit, mHM represents different hydrological processes. First, canopy interception is simulated, followed by snow accumulation and melt, which are implemented using a degree-day routine. Incoming water from rainfall and snowmelt then enters a multilayer soil/root zone, where a power-law function, adapted from the HBV model, partitions it between soil moisture storage and percolation. Evapotranspiration is calculated from potential ET and reduced by soil-water stress, weighted by the root fraction in each soil layer. Runoff generation is divided into three pathways: (i) fast interflow, triggered when unsaturated storage exceeds a threshold; (ii) slow interflow, representing steady drainage from the same store; and (iii) baseflow from a lower groundwater reservoir, treated as a linear store. The combined flows are routed through the river network using the time-adaptive Muskingum–Cunge scheme (Thober et al., 2019). Full algorithmic details and mHM parameterizations can be found at www.ufz.de/mhm.

The hydrological fluxes of the lumped and landscape-explicit model structures are based on the mHM. From the mHM model, the total outflow from the soil ( mm ha-1 day-1), total baseflow from groundwater ( mm ha-1 day-1), and the total groundwater recharge ( ha-1 day-1) from all grid cells are calculated as follows:

, (S1)

, (S2)

, (S3)

where the superscript “i” indicates the grid cell ith, n is the total number of grid cells in the catchment, t (day) is time, , , , and (mm ha-1 day-1) are fast interflow, slow interflow, baseflow, and groundwater recharge at the grid cell level, respectively, simulated from the mHM model, and (m2) is the grid cell area.

The average catchment scale water storage in the soil ( mm)) and groundwater ( mm)) from mHM are:

, (S4)

, (S5)

where x3 and x5 (mm) are water storage from different soil zones (simulated from mHM), and x6 (mm) is groundwater storage (simulated from mHM).

***Lumped model structure:***

In the lumped model structure (Fig. 1a), QHS, QRCH, QGW (mm ha-1 day-1) are the same as , , and , respectively. Total outflow ( mm ha-1 day-1) from the catchment is:

, (S6)

The storage of the hillslope ( mm) and groundwater zone ( mm) are:

, (S7)

, (S8)

where and (mm) are the initial water storage in the hillslope and groundwater zone, respectively.

***Landscape-explicit model structure:***

In the landscape-explicit model structure (Fig. 1b), QHS (mm ha-1 day-1) needs to be adjusted to account for the upland area fraction. As the area fraction of the upland is fUL (-), therefore, flow out of the upland is:

, (S9)

Groundwater flow to the stream ( mm ha-1 day-1) and to the riparian zone ( mm ha-1 day-1), considering the upland area fraction () and the fraction of groundwater flow to riparian zone (, are:

, (S10)

, (S11)

Therefore, the amount of inflow to the riparian zone is:

= , (S12)

To ensure a consistent streamflow simulation with the mHM model, we assumed that in the riparian zone, inflow equals outflow. Therefore, the total outflow ( mm ha-1 day-1) from the catchment is:

, (S13)

Streamflow in the lumped (Eq. S6) and landscape-explicit (Eq. S13) model structures are identical. Water storage in the upland and groundwater zone are the same as Eqs. S7-S8 while the water storage in the riparian zone ( mm) is:

, (S14)

where (mm) is the initial water storage in the riparian zone.

# Text S2. Model performance metrics

In addition to the KGE that was used for model calibration, we also evaluated the performance of behavioural simulations using the Nash–Sutcliffe efficiency (NSE, Nash and Sutcliffe, 1970), relative bias (BIAS), and R-squared (R2):

, (S15)

, (S16)

, (S17)

where and the observed and simulated streamflow (or stream DOC concentration), respectively, k is the index, n is the number of observations, and are the mean of observed and simulated values, respectively.

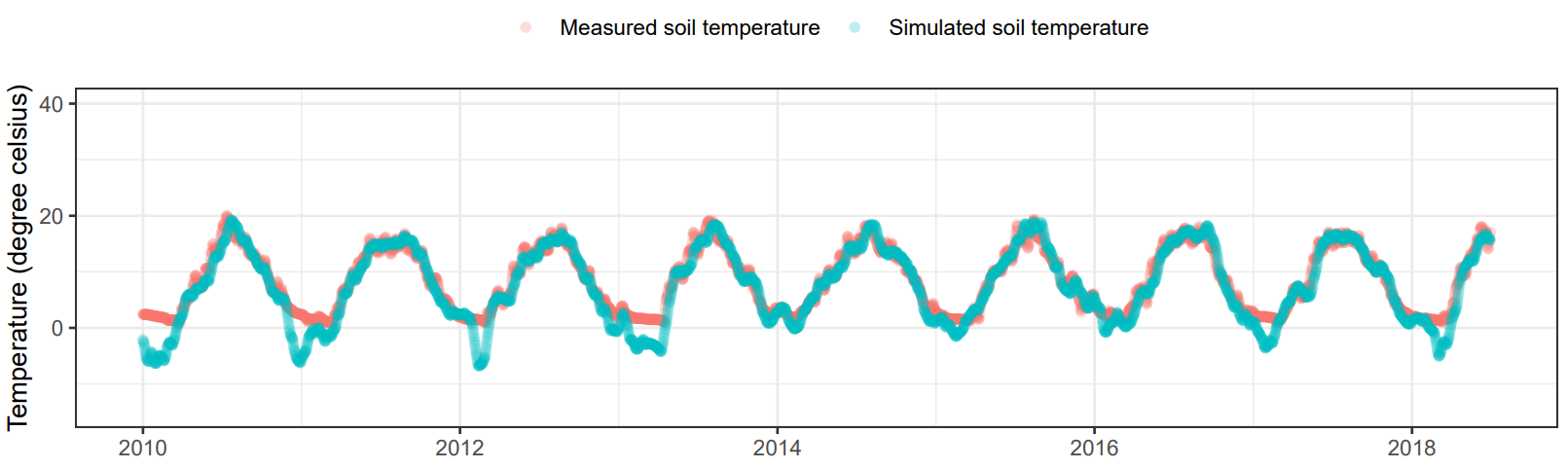


Figure S1. Measured soil temperature (at a 50 cm depth near the study area (Station ID 00656; German Weather Service) was compared with the calculated temperature using Equation (3) (with n = 35) and air temperature data from the Hassel catchment as an example. Measured soil temperature can be obtain at <https://opendata.dwd.de/climate_environment/CDC/observations_germany/climate/daily/soil_temperature/> (last accessed: 7 June 2025).

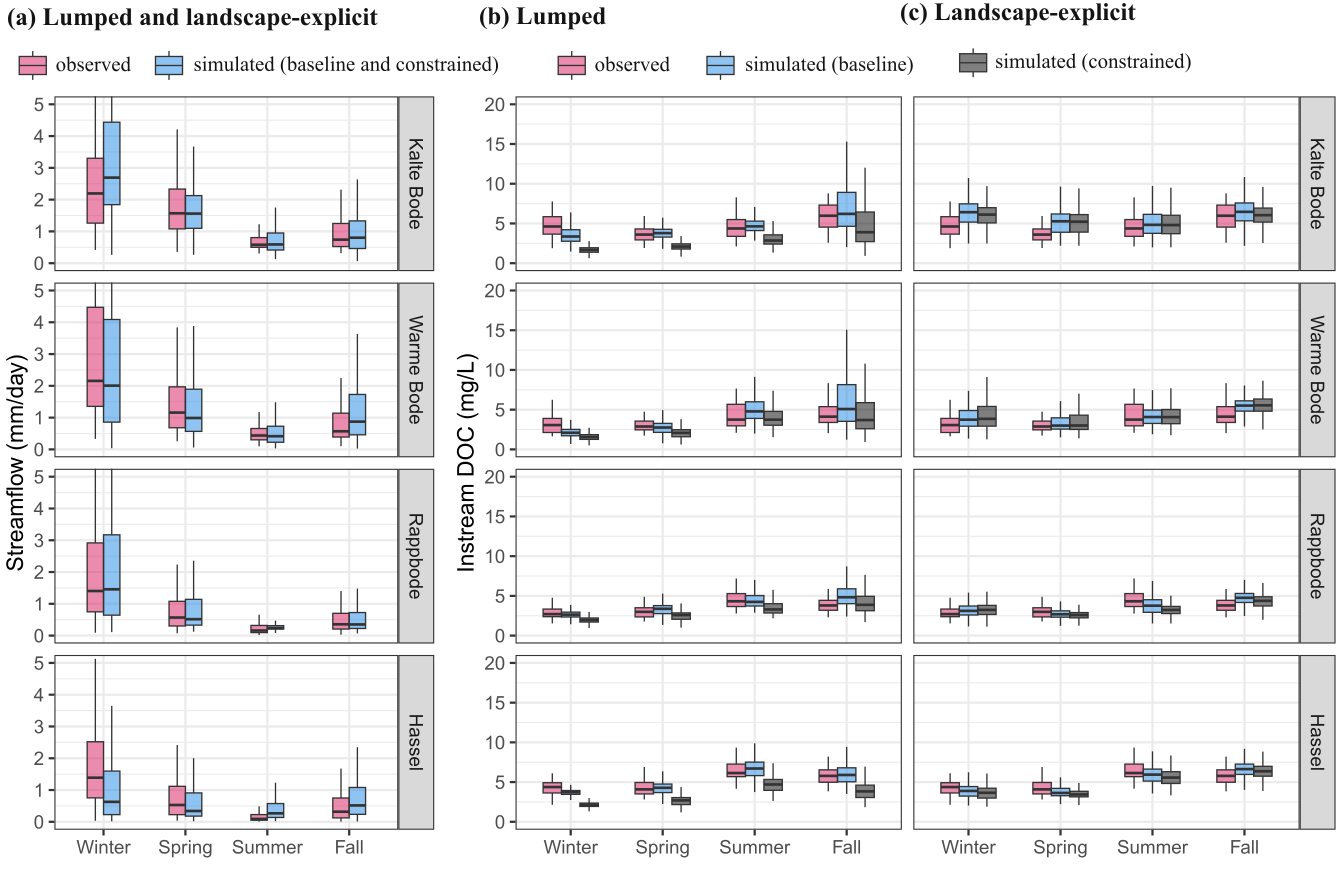


Figure S2. Boxplots of observed (obs) and simulated (sim) (a) streamflow and (b-c) stream DOC concentrations by seasons (Winter: December to February; Spring: March to May; Summer: June to August; Fall: September to November) in the four catchments and with lumped and landscape-explicit model structures under the baseline and constrained calibrations. Data were taken from both calibration and validation periods.

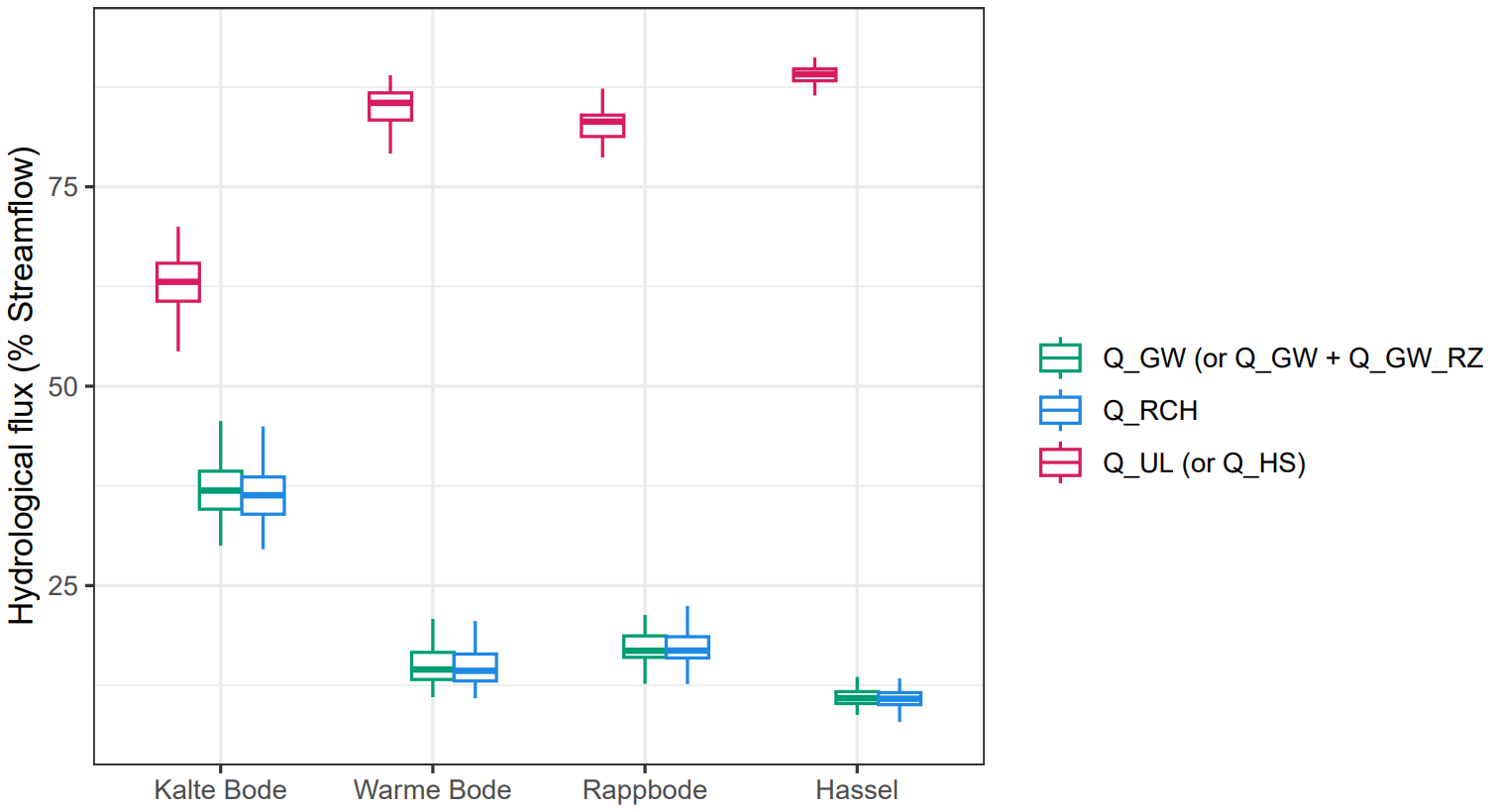


Figure S3. Boxplots of annual average hydrological fluxes (in percentage of streamflow) for both calibration and validation periods from 30 behavioural models of each catchment (baseline calibration). QUL (or QHS) and QGW (mm/year) are outflows from the upland (or hillslope when referring to the lumped model structure) and from groundwater to stream, respectively. QRCH (mm/year) is the groundwater recharge. The sum of QGW and QGW\_RZ is the total outflow from groundwater to stream and groundwater to riparian zone in the landscape-explicit model.

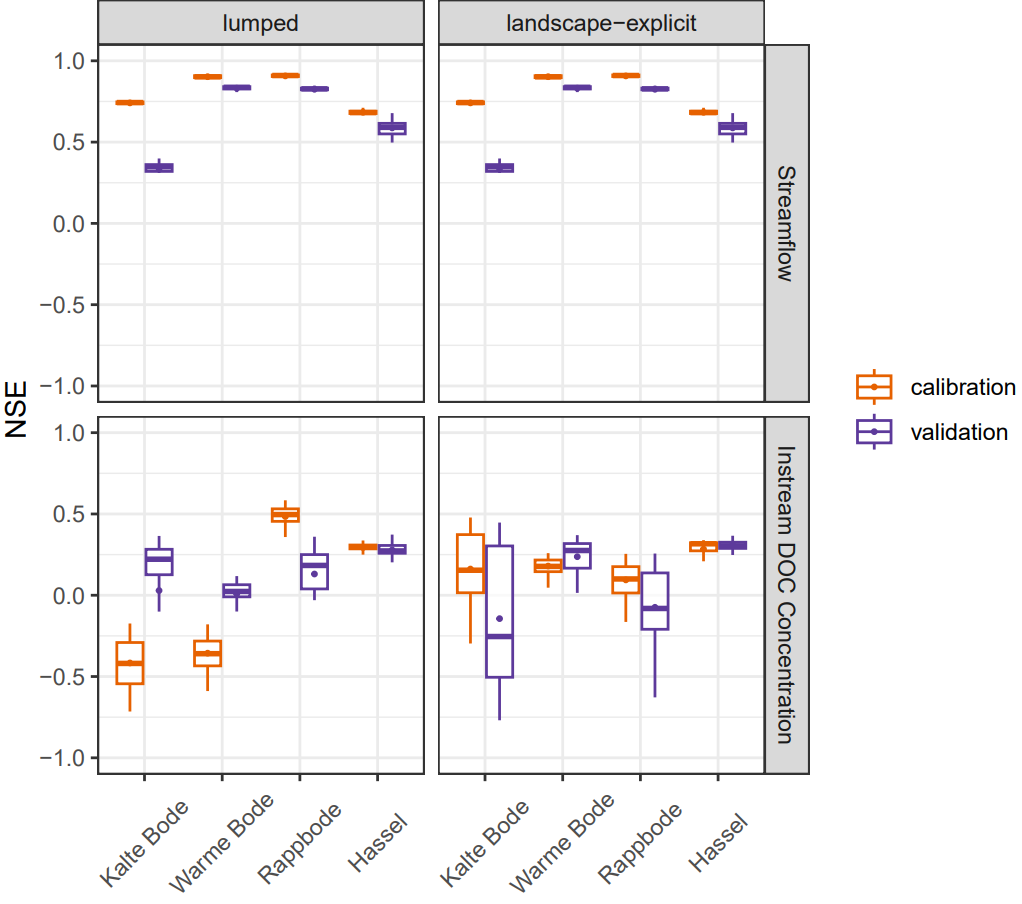


Figure S4. Boxplots of the NSE from the 30 behavioural simulations for streamflow and stream DOC under the baseline calibration. The dot represents the mean value. Note that streamflow results are identical because hydrological modelling preceded the differentiation of model structures in DOC modelling.

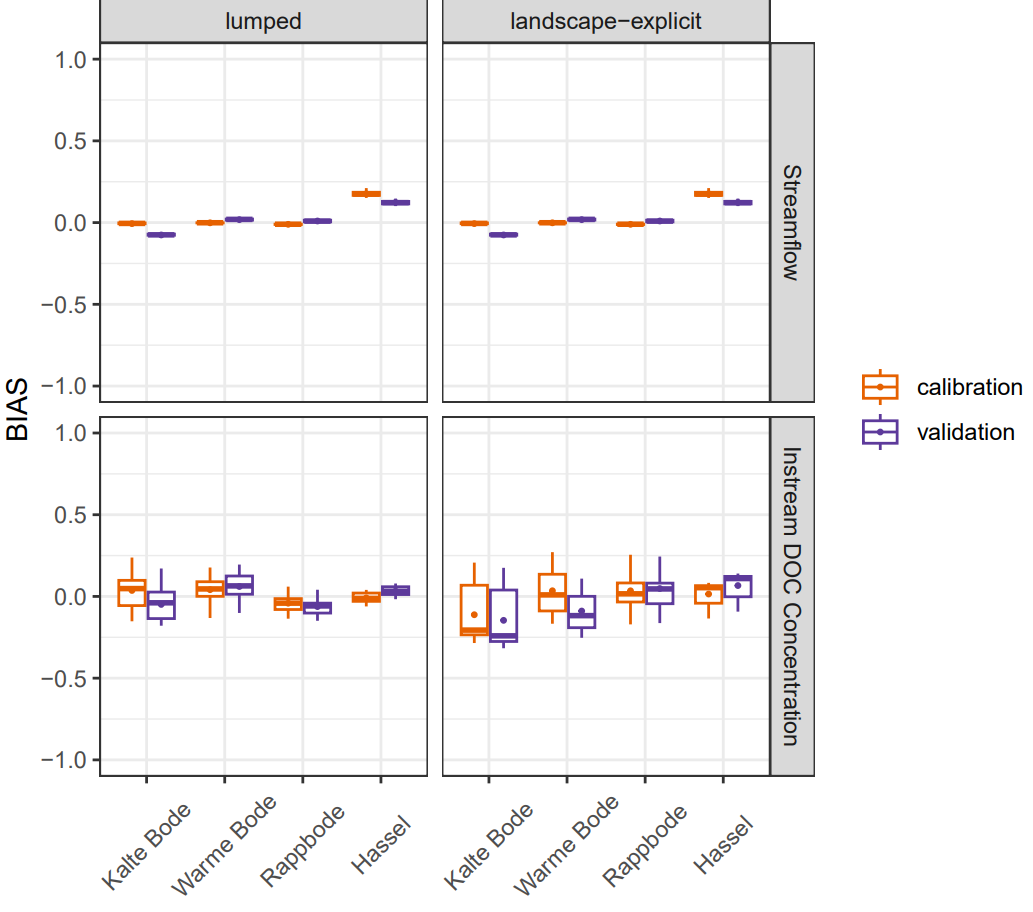


Figure S5. Boxplots of the BIAS from the 30 behavioural simulations for streamflow and stream DOC under the baseline calibration. The dot represents the mean value. Note that streamflow results are identical because hydrological modelling preceded the differentiation of model structures in DOC modelling.

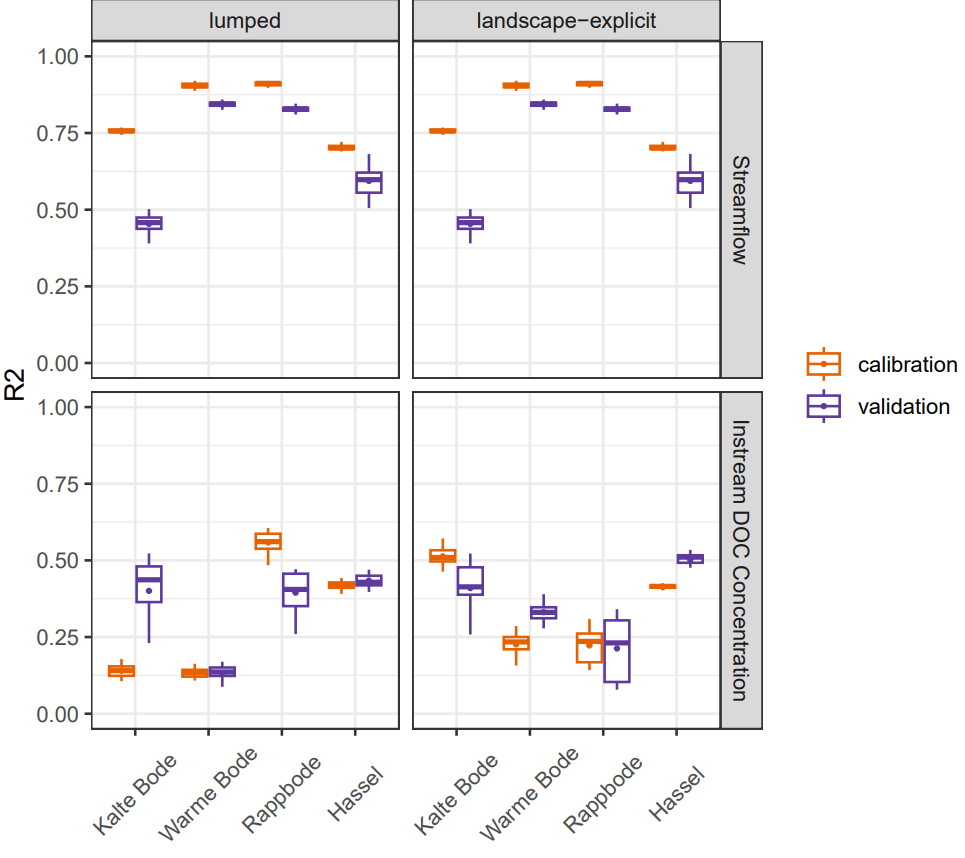


Figure S6. Boxplots of the R2 from the 30 behavioural simulations for streamflow and stream DOC under the baseline calibration. The dot represents the mean value. Note that streamflow results are identical because hydrological modelling preceded the differentiation of model structures in DOC modelling.

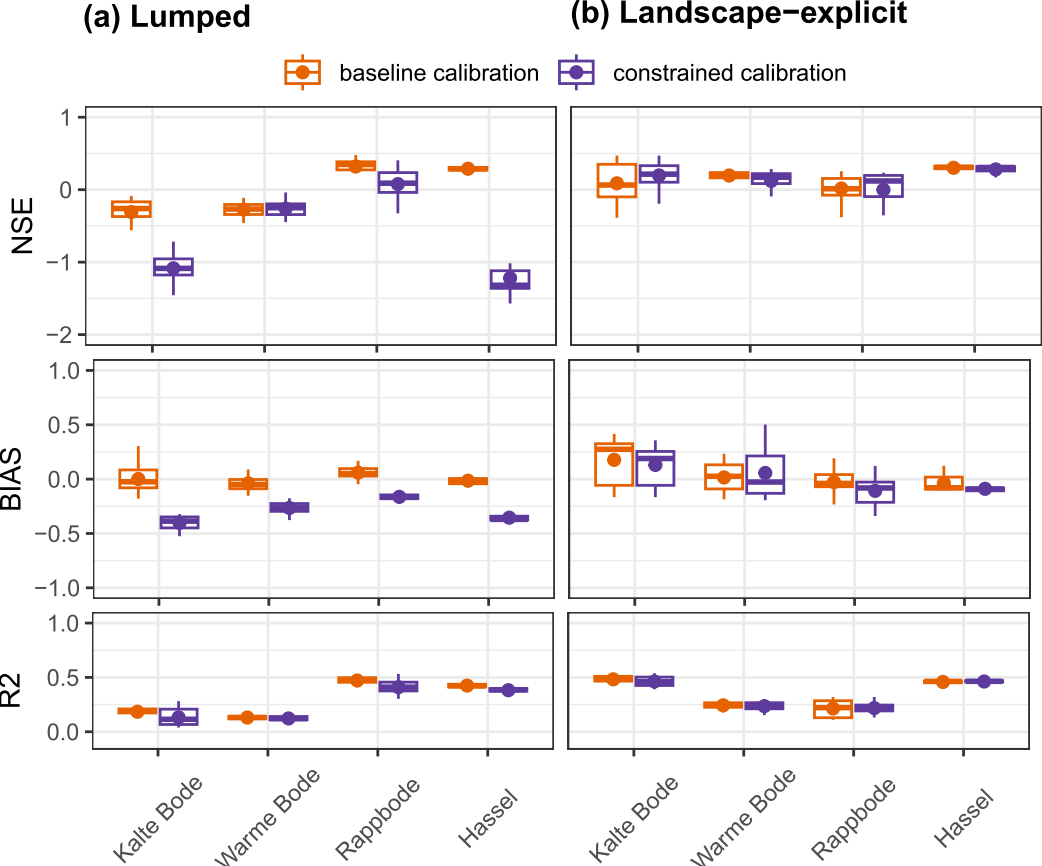


Figure S7. Boxplots of the NSE, BIAS, and R2 from 30 behavioural simulations for stream DOC under the baseline calibration and constrained calibration. The dot represents the mean value. The NSE, BIAS, and R2 were calculated for both calibration and validation periods.

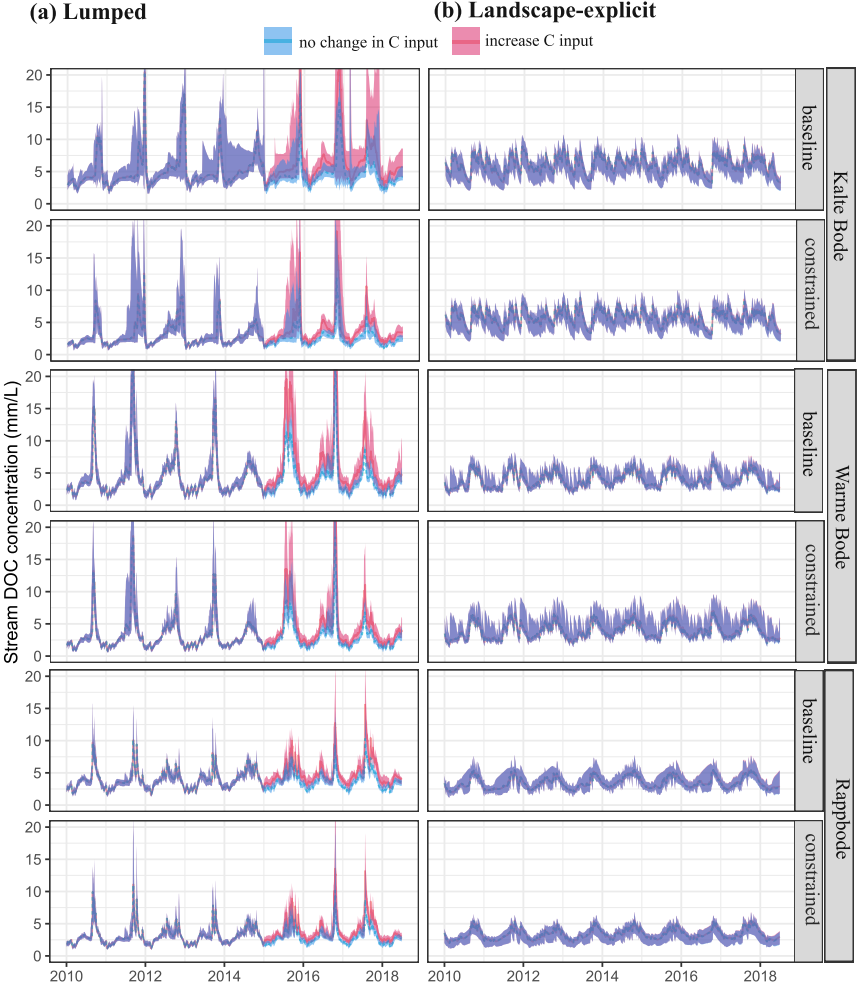


Figure S8. Simulated stream DOC concentrations in the Kalte Bode, Warme Bode, and Rappbode catchments with increasing C input by 5 kg/ha for the period 2015-2018 (a) in the hillslope of the lumped model structure and (b) in the upland of the landscape-explicit model structure and (b).

# References

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