Supporting information for:

Data-driven system dynamics model for simulating water quantity and quality in peri-urban streams

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Supplementary figures

Figure S1 shows an example of developed System Dynamic module within the STELLA software environment.

Figure S2 to S4 shows the type and extent of sewer network (S2), location of separated sewer outlets, CSOs outlets and water abstraction wells (S3), and the impervious data (S4) in the investigated catchment.

Figure S5 shows the Manning´s number vs. stream water flow scatterplot in the investigated catchment.

Figure S6 displays the regression model air-water temperature used for the natural flow and separated sewer system temperature component.

Figure S7 displays the water flow simulation results, all reaches.

Figure S8 displays the stream depth simulation results, all reaches.

Figure S9 shows the Combined Sewer Overflow (CSOs) results.

Figure S10: displays the water flow simulation results, Donse tributary.

Figure S11 displays the Simulation results for DO daily average concentration expressed in % DO sat (Parallelvej station, see Fig.1)

Figure S12 displays the nitrate concentration results (deterministic solution for reaches Ådalsvej and Nivemølle, see Fig. 1)

Figure S13 displays the ammonium concentration results (deterministic solution for reaches Ådalsvej and Nivemølle, see Fig. 1)

Figure S14 displays the orthophosphate concentration results (deterministic solution for reaches Ådalsvej and Nivemølle, see Fig. 1)

Figure S15 displays the suspended Chlorophyll A concentration results, (deterministic solution for reaches Ådalsvej and Nivemølle, see Fig. 1).

Figure S16 displays the forcing data (nutrients and Chla) used as input for the simulation shown in S12-S15 and Fig. 7.

Figure S17 shows the results of the Rainfall-Runoff model sensitivity testing (Nivemølle).

Figure S18 shows the results of sensitivity test for the DO concentration simulation (Parallelvej).

Supplementary tables:

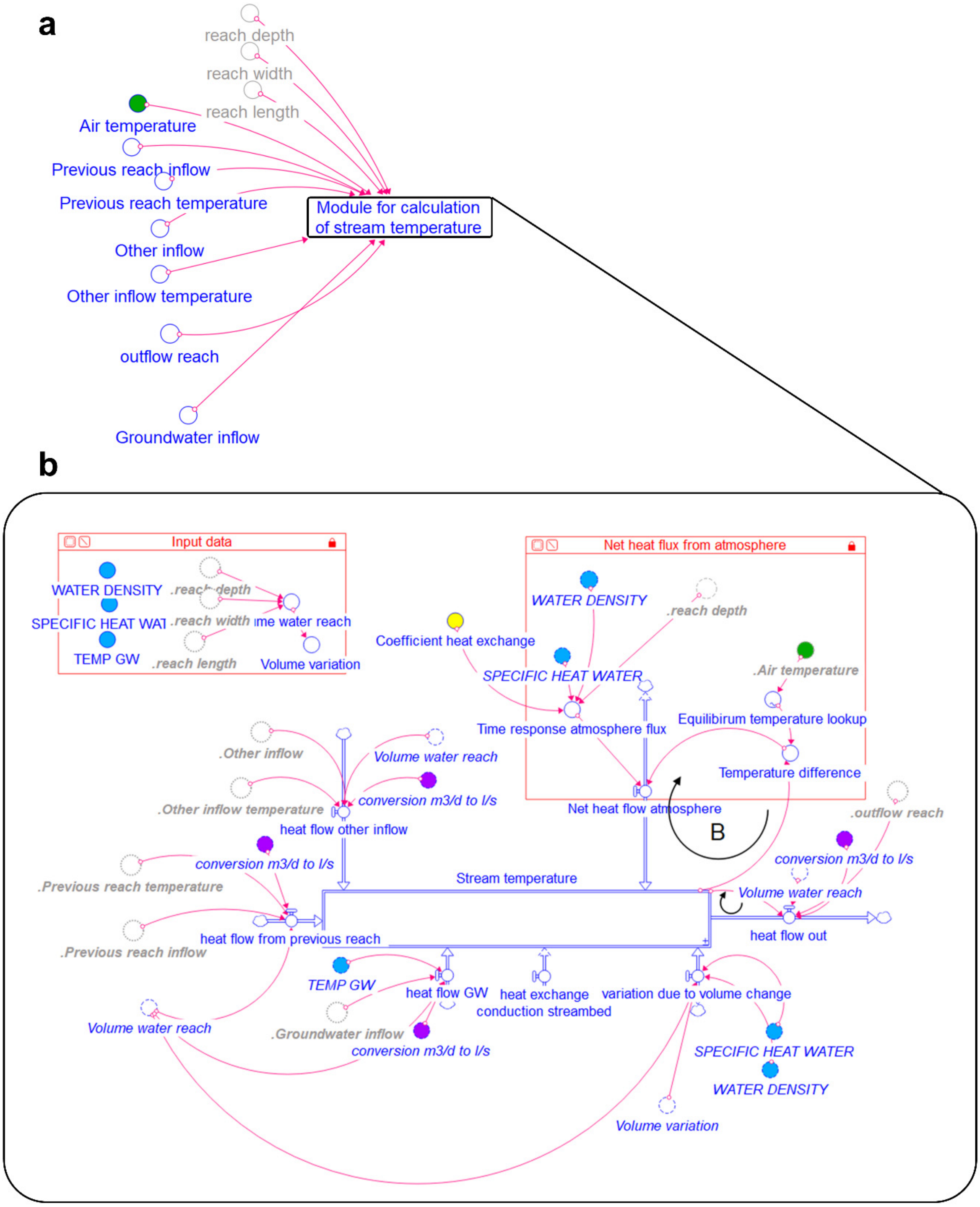
Table S1 provides a summary of available input and monitoring data for the simulated peri-urban catchment

Table S2 provides an overview of all input data, type, frequency range and data source

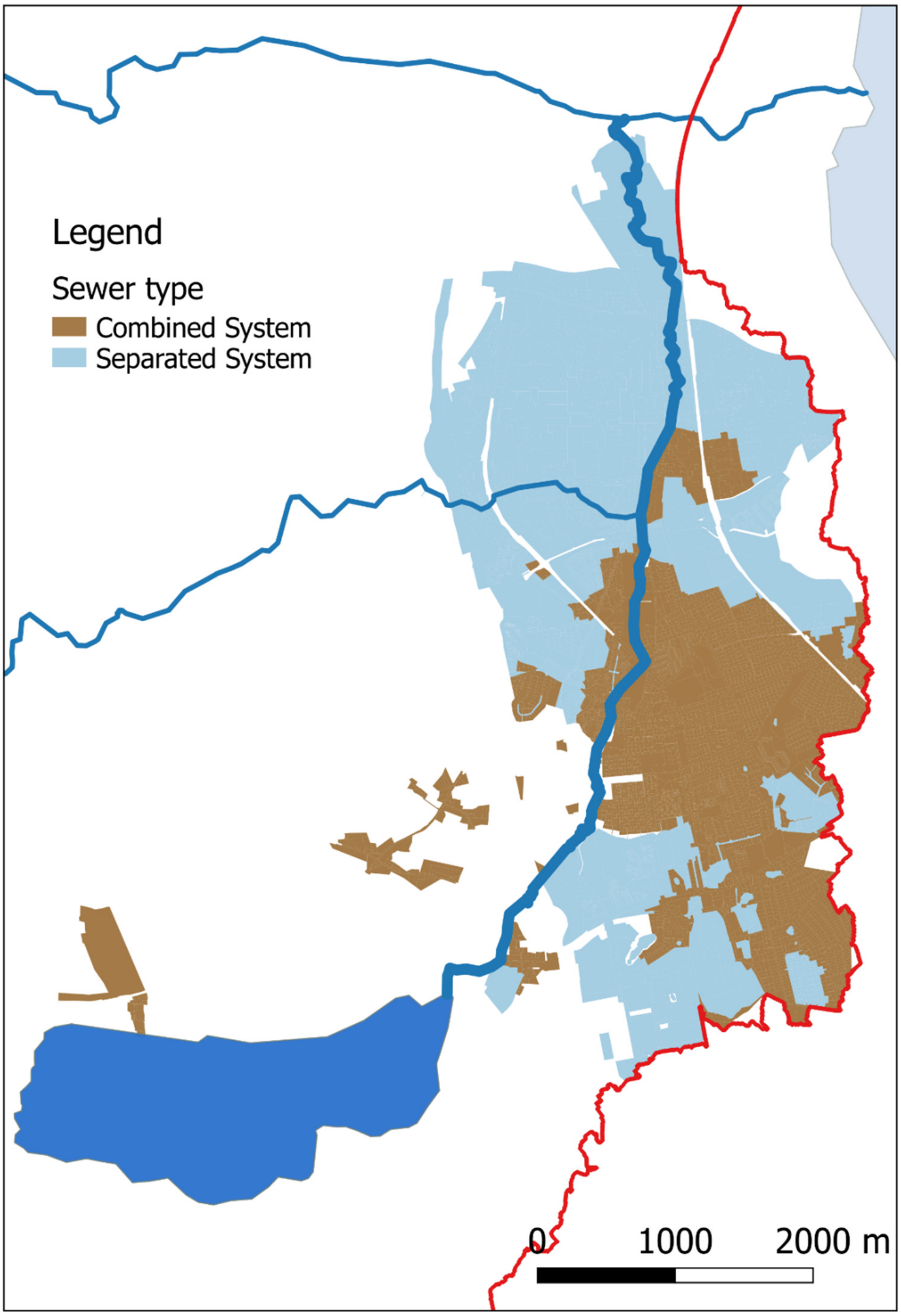
Table S3 gives the quantitative values for the Model performance rating for Nash-Sutcliffe Efficiency (NSE), Percent BIAS (PBIAS) and RMSE-observations standard deviation ratio (RSR).

Table S4 shows all model parameters and references.

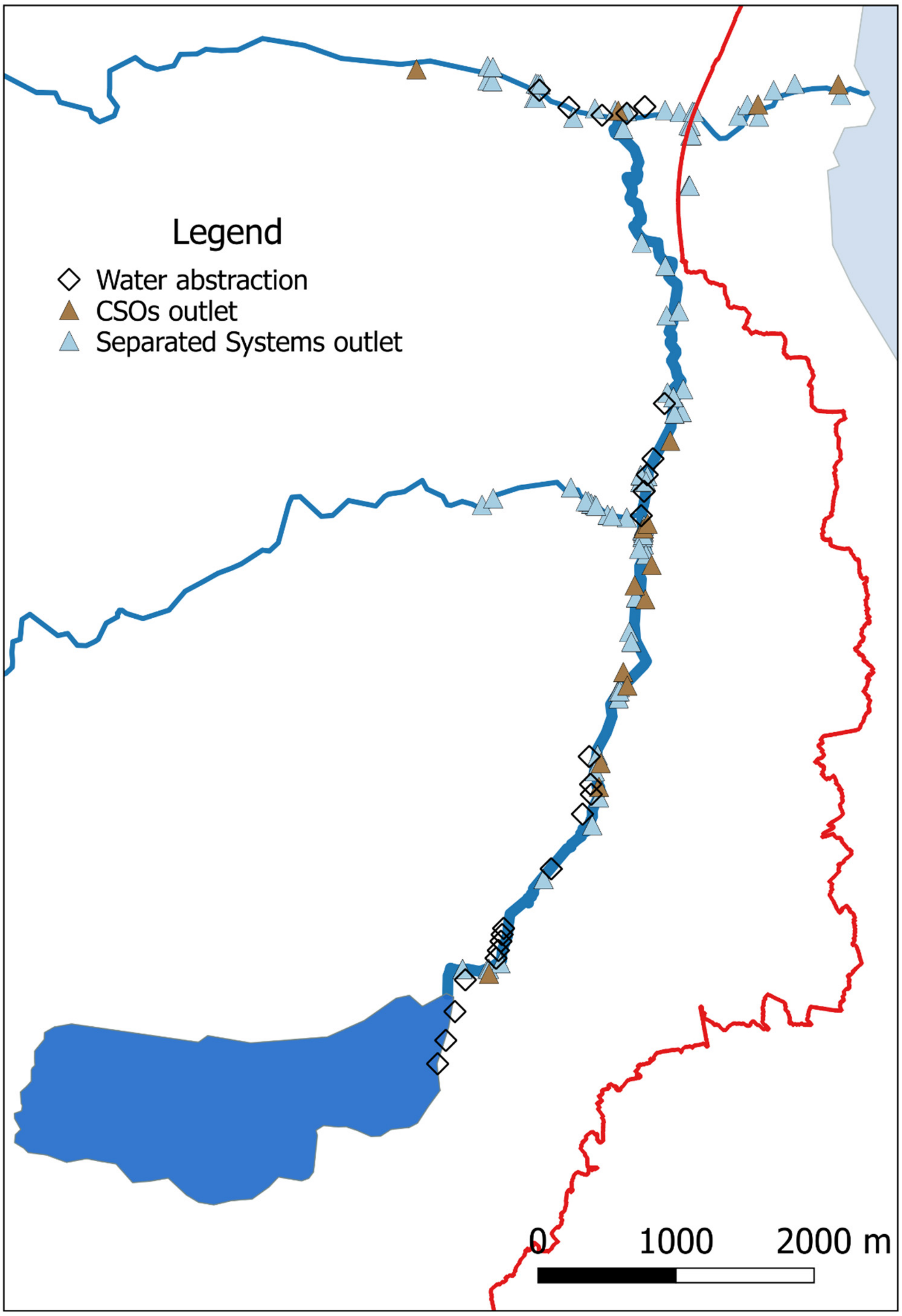
Table S5 and S6 shows the input data distribution for the MC simulations carried out for the dissolved oxygen concentration and physico-chemical parameters respectively.



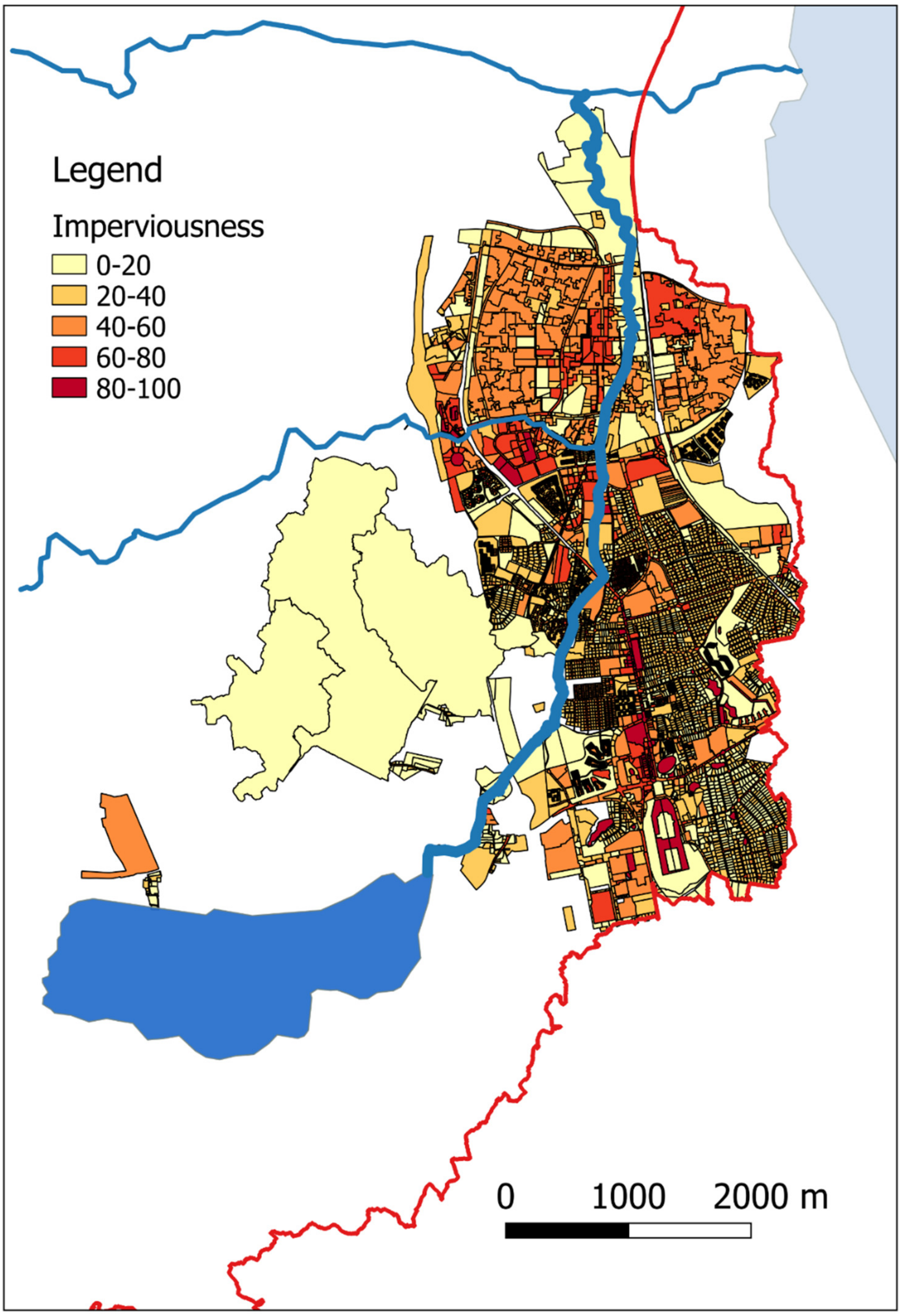
SI Figure S1. Example for an SD module developed for simulating stream temperature. The module is comprised of a) the parameters used for linkage to other components and/or modules within of the overall system; and the actual module, showing b) the detailed structure. The black arrow (loop B) demonstrates a balancing feedback loop for the heat exchange at the interface stream/atmosphere regulating water temperature to an equilibrium with air temperature.



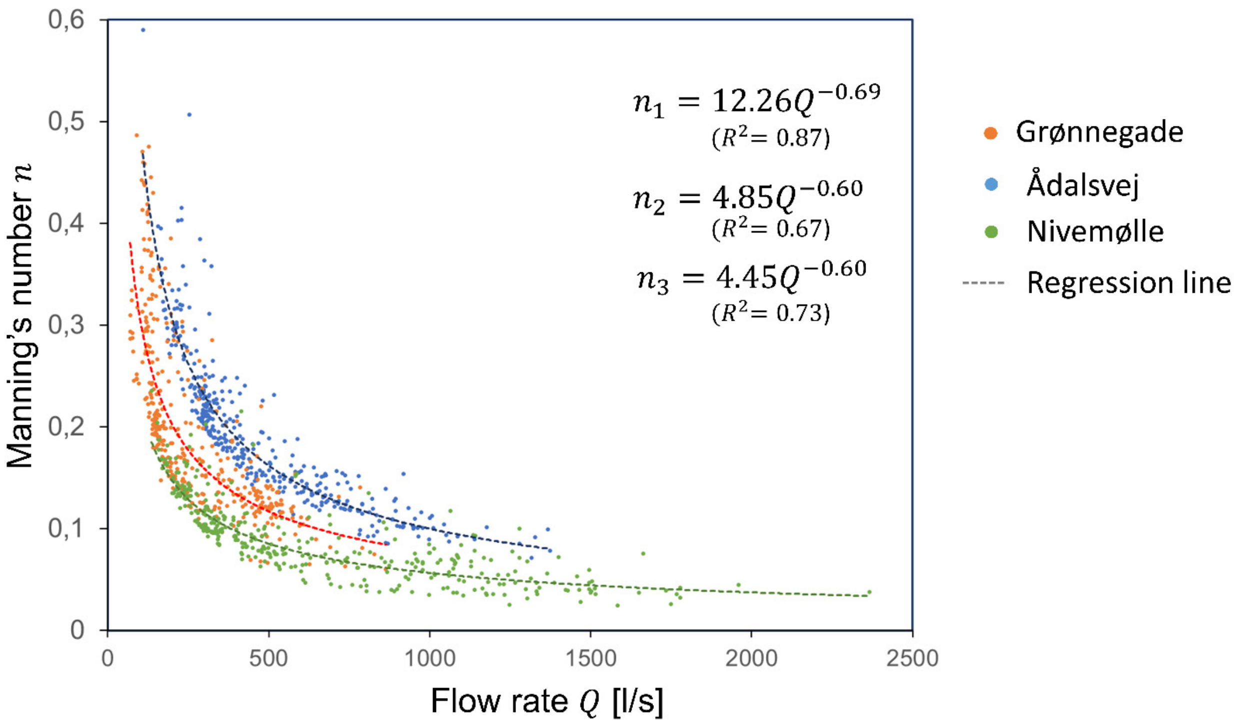
SI Figure S2. Sewer network extent and type for the Usserød catchment (NOVAFOS, 2020).



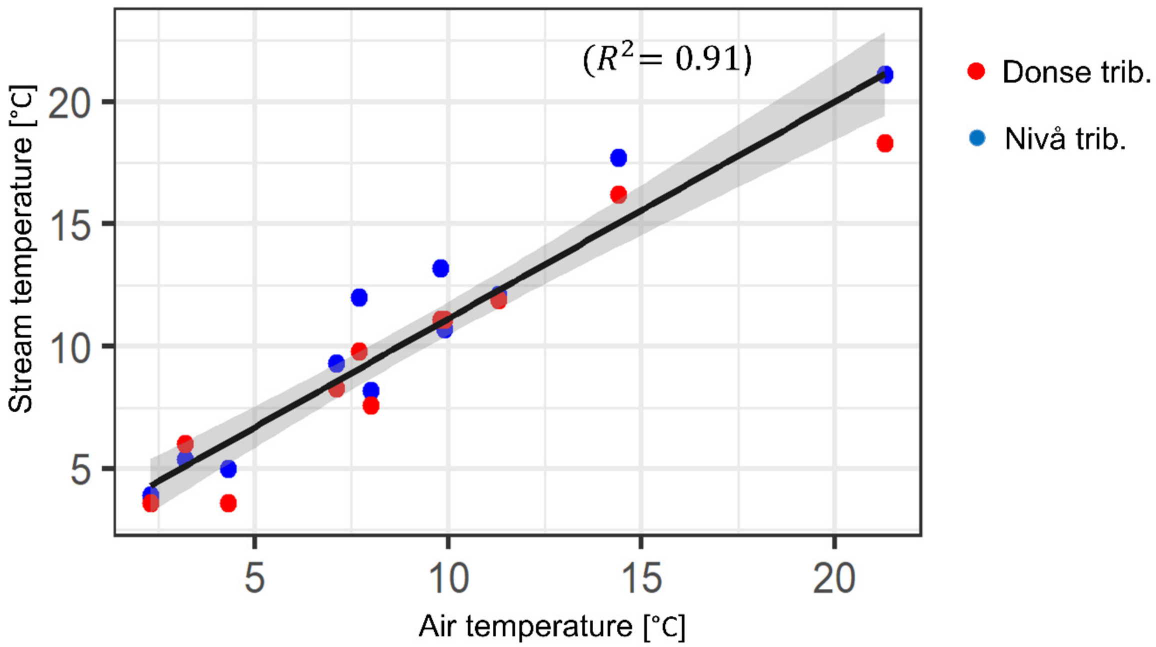
SI Figure S3. Locations for documented water abstraction, separate systems outlets and combined sewer overflows for the Usserød catchment (Danmark Miljøportal, 2020.; NOVAFOS, 2020)



SI Figure S4. Imperviousness distribution data for the Usserød catchment (NOVAFOS, 2020).



SI Figure S1. Scatterplot for the estimated Manning's number vs. flow rate measured at the outlet of the three modelled reaches in the catchment (Grønnegade: orange; Ådalsvej: blue; Nivemølle: green). Results shown only for calibration year 2017. The Manning's number is estimated using the water depth measurement and assuming a simplified rectangular cross-section profile and low depth. See Appendix A for details.



SI Figure S6. Linear regression model for the water temperature estimation of the natural water and urban system components. Data from Lemaire (2021) measured in Donse and Nivå tributaries dominated by non-urban inflows (i.e. no WWTP effluents). The grey shaded area corresponds to the 95% CI for the regression model.

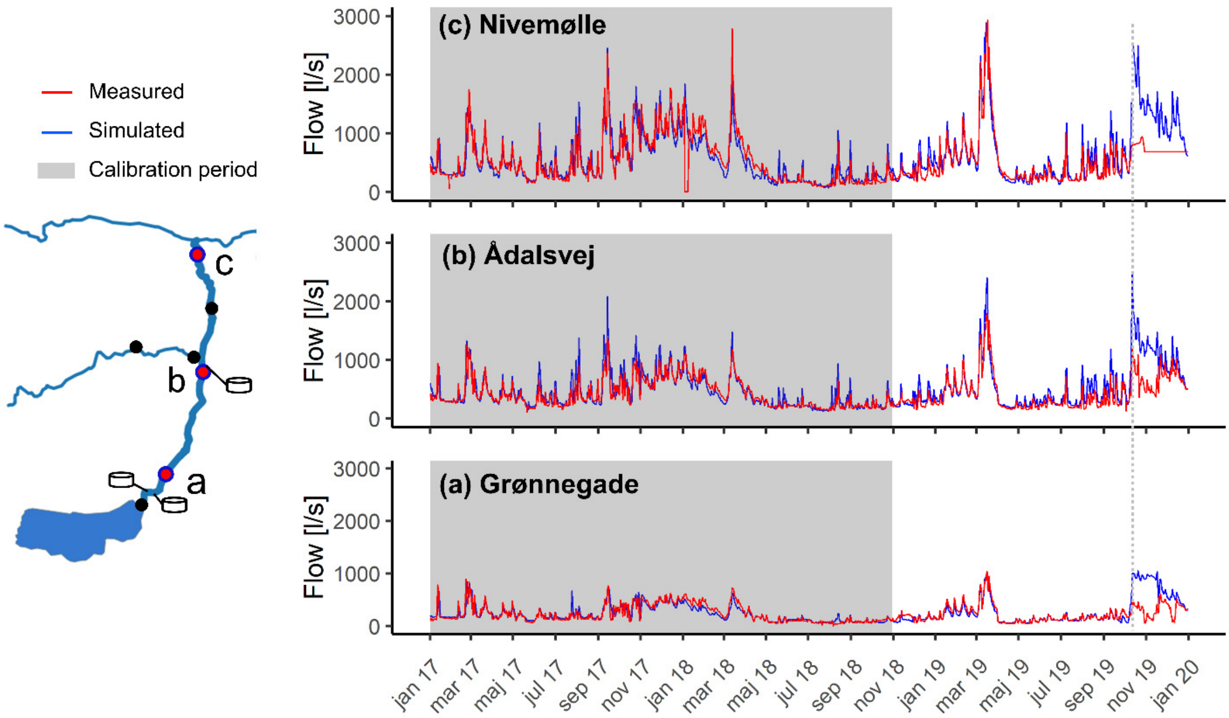


Figure S7. Flow simulation results (blue line) compared to continuous monitoring station measurements (red line) for all three Usserød stream reach outlets: Grønnegade (a), Ådalsvej (b) and Nivemølle (c) (compare Fig. 2). The grey ribbon shows the calibration period; the grey dashed line marks an event of flooding of the stream channel banks in Grønnegade reach.

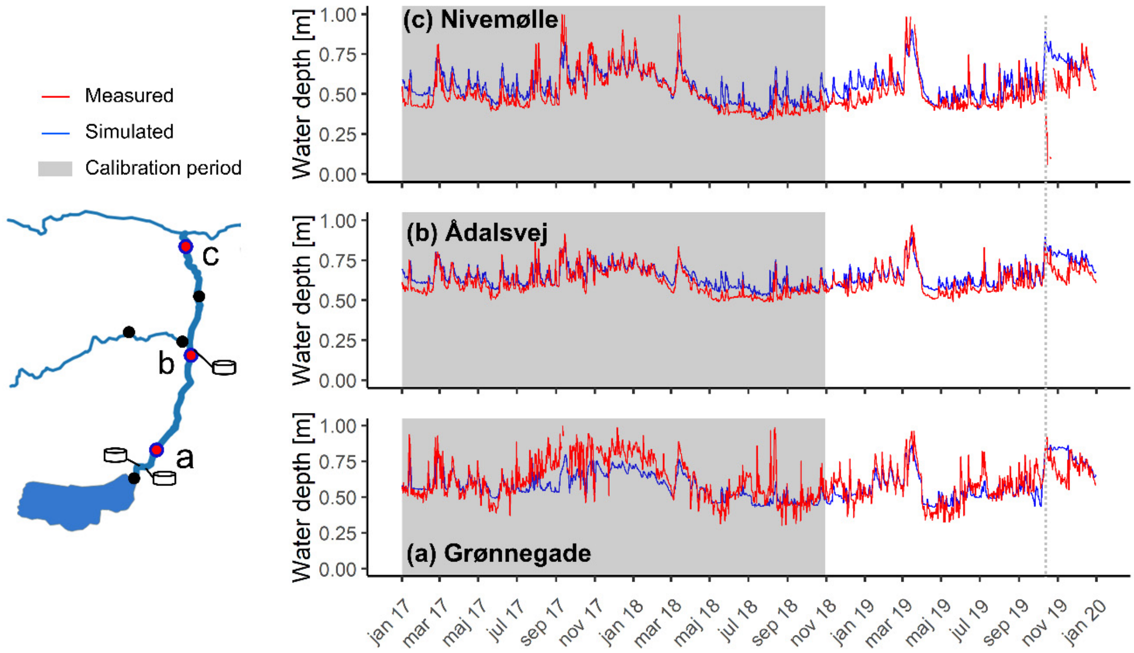


Figure S8. Water depth simulation results (blue line) compared to continuous monitoring station measurements (red line) for all three Usserød stream reach outlets: Grønnegade (a), Ådalsvej (b) and Nivemølle (c). The grey ribbon shows the calibration period; the grey dashed line marks a flooding of the stream channel banks in Grønnegade reach.

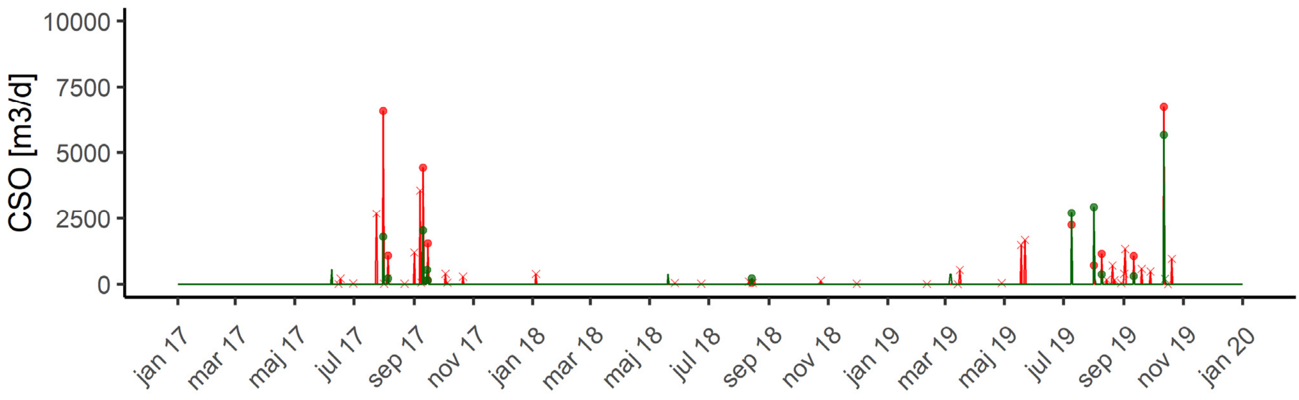


Figure S9. Combined Sewer Overflow events in Ådalsvej reach. Simulated events (green) are compared to measured events (red). Round markers pinpoint an event well captured, while cross markers indicate an event not captured on a daily basis. Total number of events captured by the model based on a simple assumption (basin with non linear flow): 11/49.

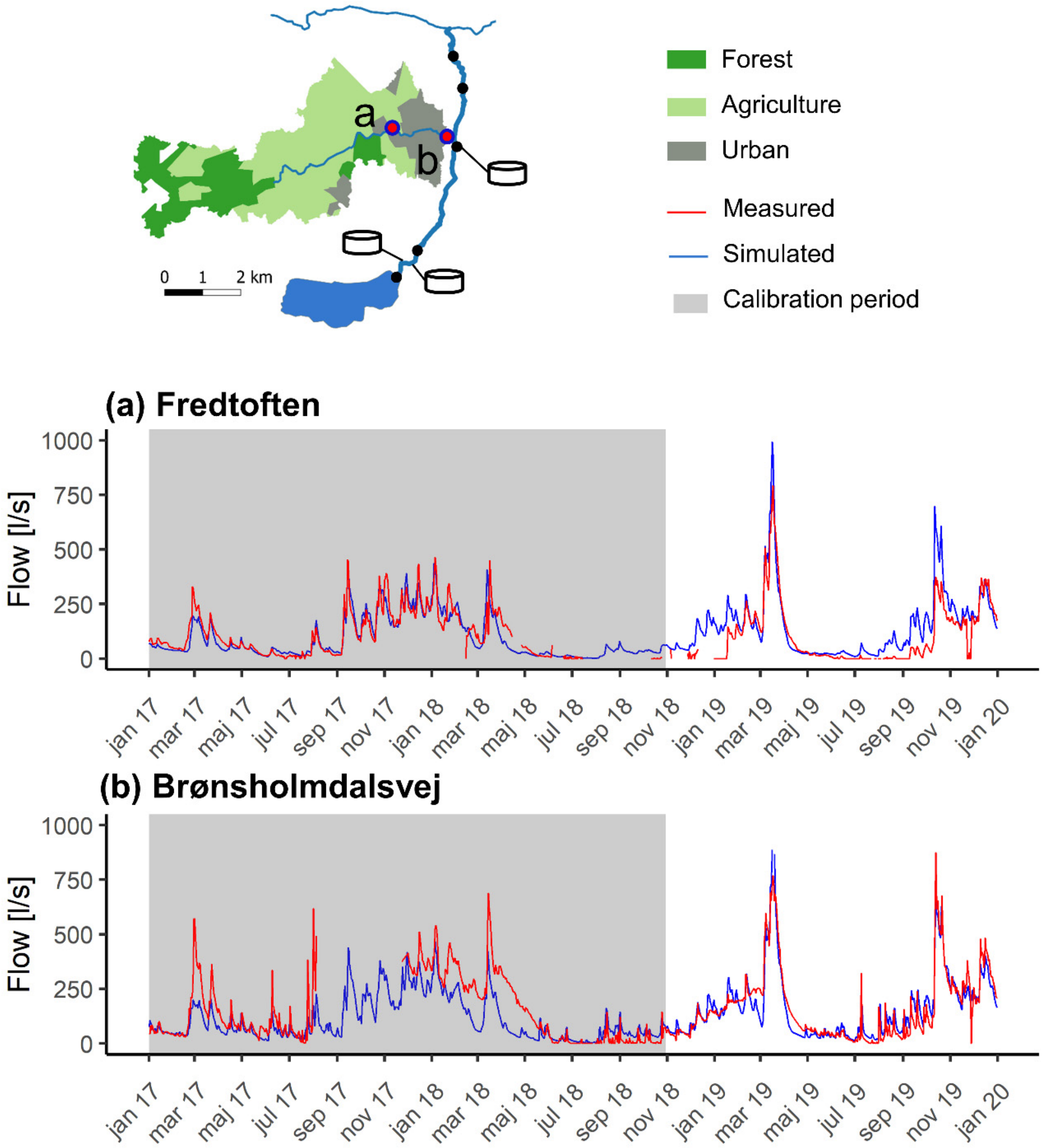


Figure S10. Flow simulation results (blue line) compared to continuous monitoring station measurements (red line) at two points, Fredtoften and Brønsholmdalsvej, in the Donse Tributary.

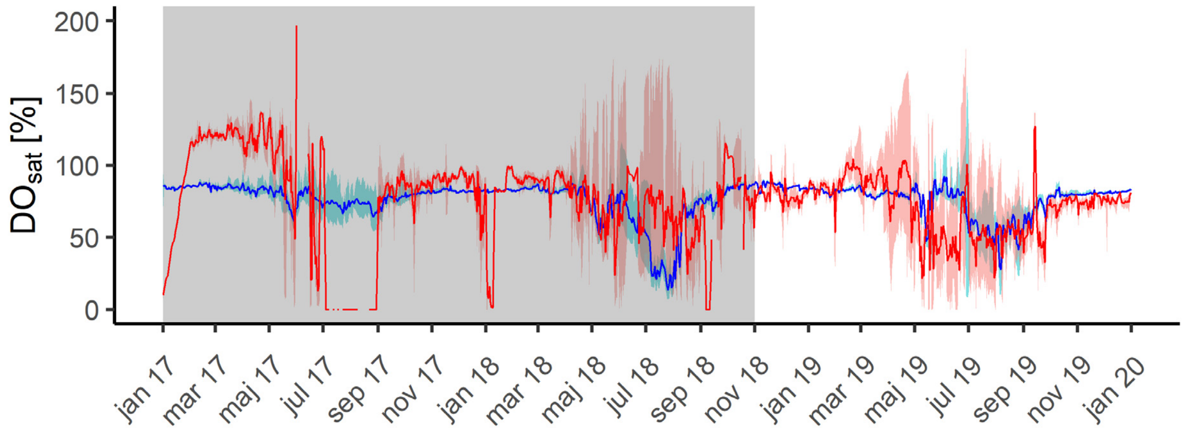


Figure S11. Simulation result for DO daily average concentration (blue line) compared to the online sensor data (red line) at Parrallelvej monitoring station (Fig. 2), expressed in %DO saturation. The grey ribbon indicates the calibration period. The pale blue and red shadings correspond to the amplitude of simulated and measured daily extremes respectively.

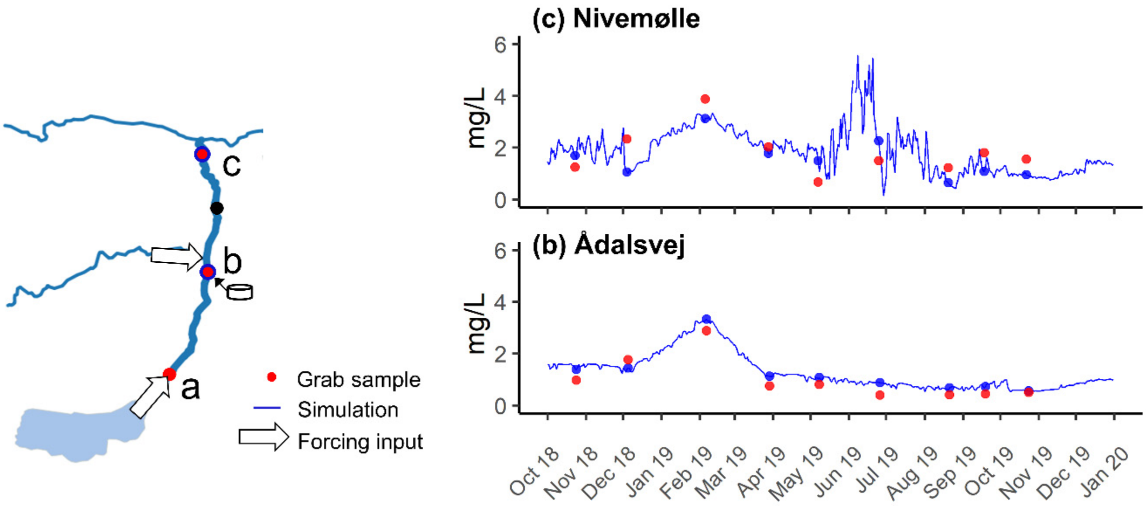


Figure S12. Simulation results (blue line) for NO3-N concentration in Ådalsvej and Nivemølle reach, compared to grab sample measurements (red circles). The corresponding daily simulation result is marked by a blue circle to facilitate the comparison. Grab sample concentrations at Grønnegade (a) and at the outlet of the tributary are combined with the estimated flow data as a forcing input (see SI Fig. S16).

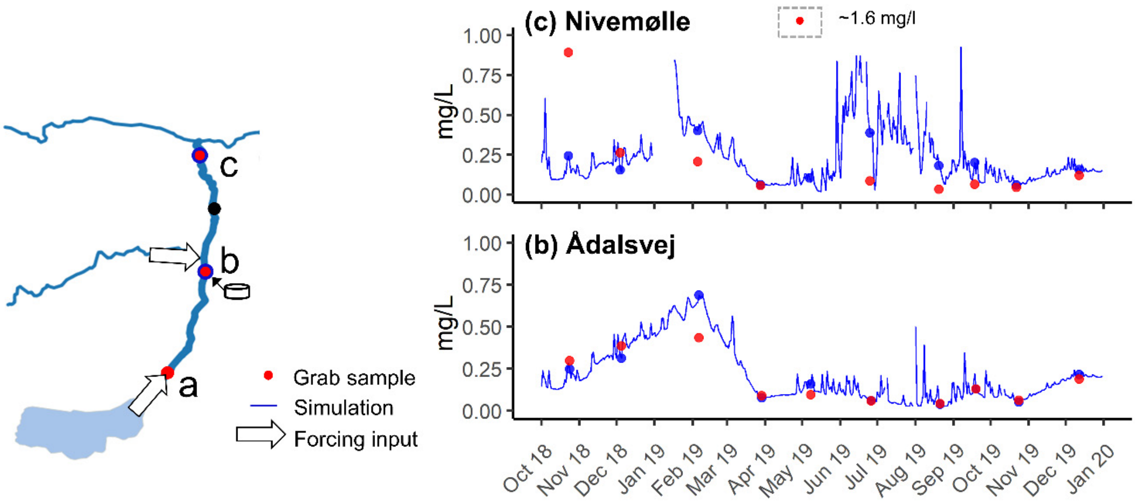


Figure S13. Simulation results (blue line) for NH4-N concentration in Ådalsvej and Nivemølle reach, compared to grab sample measurements (red circles). The corresponding daily simulation result is marked by a blue circle to facilitate the comparison. Grab sample concentrations at Grønnegade (a) and at the outlet of the tributary are combined with the estimated flow data as a forcing input (see SI Fig. S16).

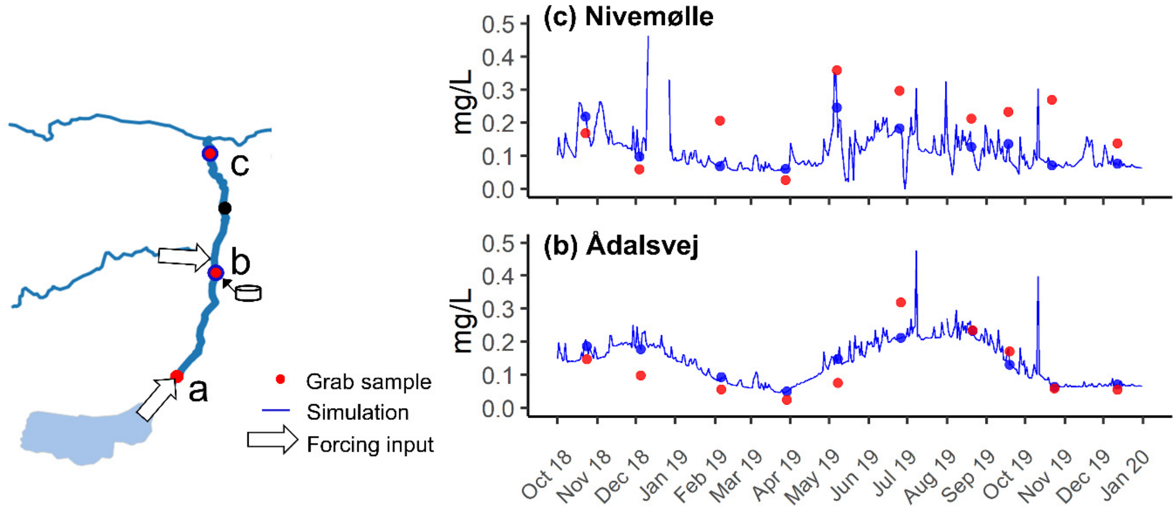


Figure S14. Simulation results (blue line) for PO4-P concentration in Ådalsvej and Nivemølle reach, compared to grab sample measurements (red circles). The corresponding daily simulation result is marked by a blue circle to facilitate the comparison. Grab sample concentrations at Grønnegade (a) and at the outlet of the tributary are combined with the estimated flow data as a forcing input (see SI Fig. S16).

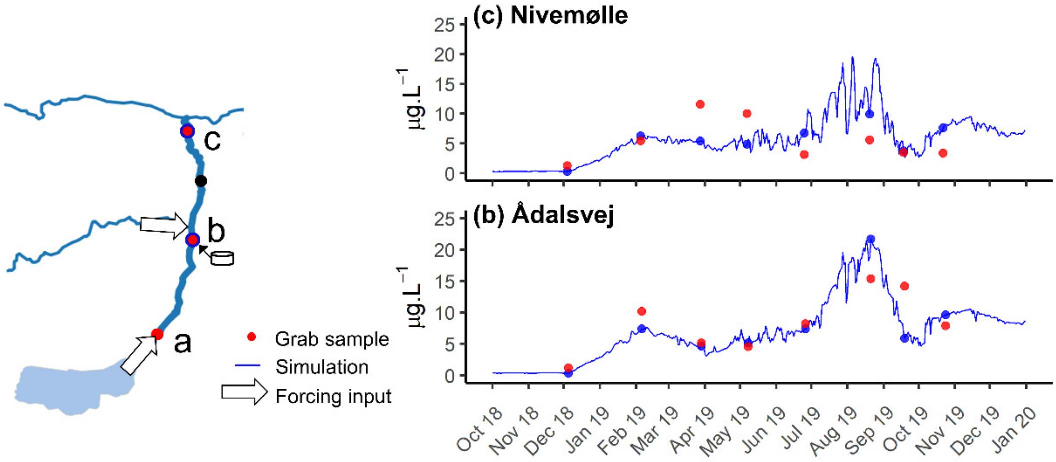


Figure S15. Simulation results (blue line) for suspended chl-a concentration in Ådalsvej and Nivemølle reach, compared to grab sample measurements (red circles). Grab sample concentrations at Grønnegade (a) and at the outlet of the tributary are combined with the estimated flow data as a forcing input (see SI Fig. S16).

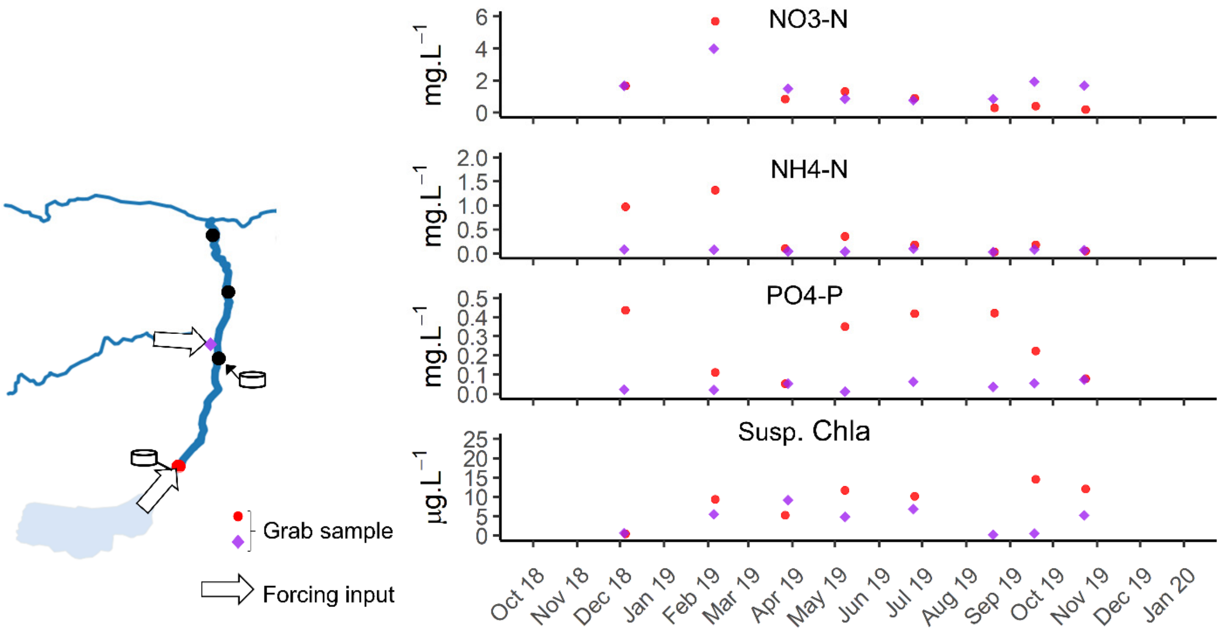


Figure S16. Forcing input concentrations at Grønnegade (red circle) and at the outlet of the tributary (purple diamond) for NO3-N; NH4-N; PO4-P and susp. Chl-a used for the simulations presented in Fig. S12-15 and Fig. 7.

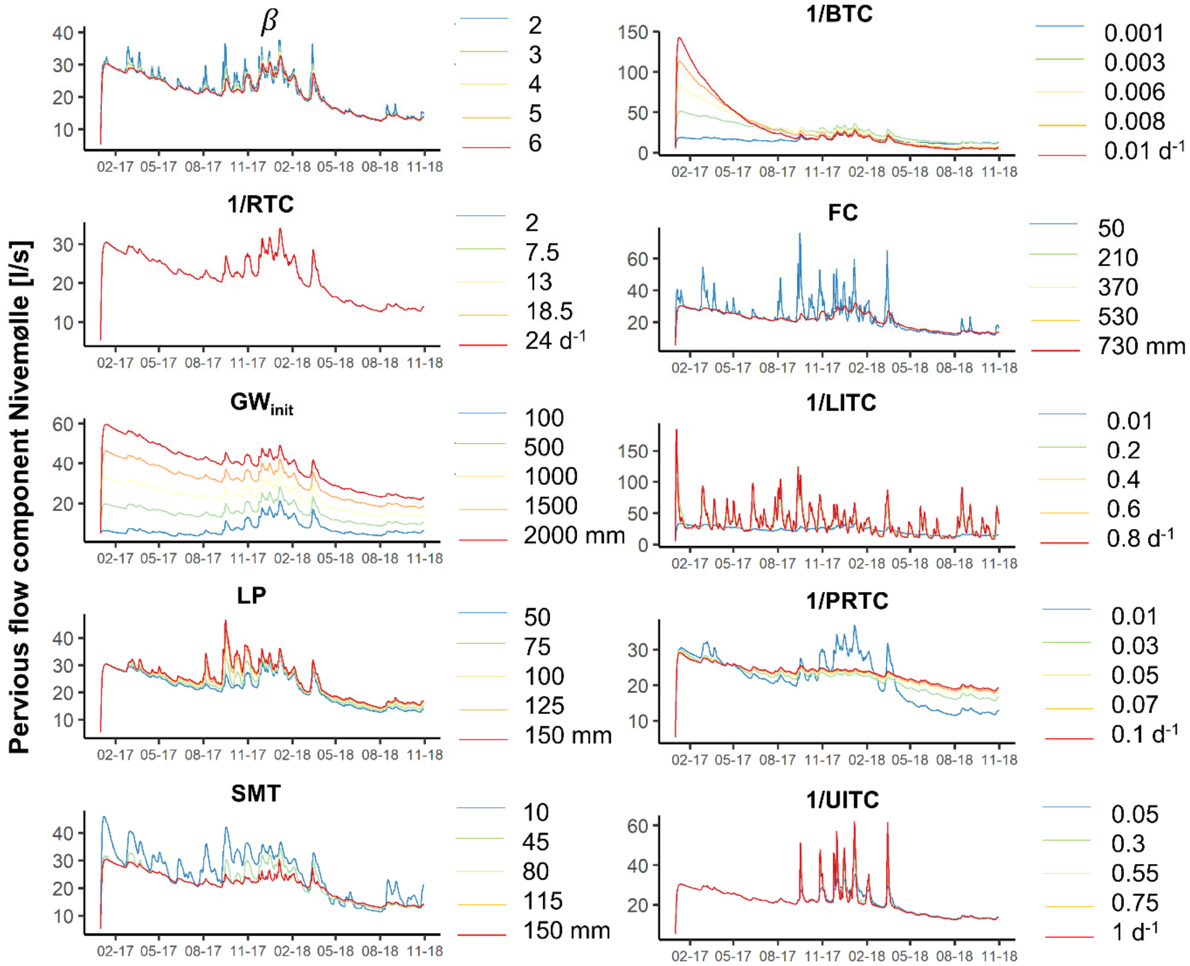


Figure S17. Rainfall-Runoff model sensitivity testing (Nivemølle station). Results are presented at a daily average time-step. Parameters range and references are given in the Table X1 below.

Table X1. Parameter ranges for the sensitivity test of the Rainfall-Runoff model

Parameter	Unit	Description	Range	Reference for range
FC	mm	Field capacity equivalent	[50–700]	Beck et al. (2016)
LP	mm	Soil moisture threshold for Potential Evapotranspiration	[50–150]*	Beck et al. (2016)
β	-	Evapotranspiration reduction factor	[1–6]	Beck et al. (2016)
SMT	mm	Soil moisture threshold – upper interflow	[10–150]*	Beck et al. (2016)
1/RTC	day^{-1}	Runoff time constant	[2–24]	Estimate
1/UITC	day^{-1}	Upper interflow rate	[0.05–1]	Beck et al. (2016)
1/LITC	day^{-1}	Lower interflow time rate	[0.01–0.8]	Beck et al. (2016)
1/PRTC	day^{-1}	Percolation rate	[0,01–0,1]	Beck et al. (2016)**
1/BTC	day^{-1}	Baseflow rate	[0.001–0.01]	Beck et al. (2016)
GWinit	mm	Deep soil moisture initial value	[100–2000]	Estimate

*: upper limit bounded by the calibrated model parameters

**: to ensure percolation rate variation within range reported by (Beck et al., 2016)

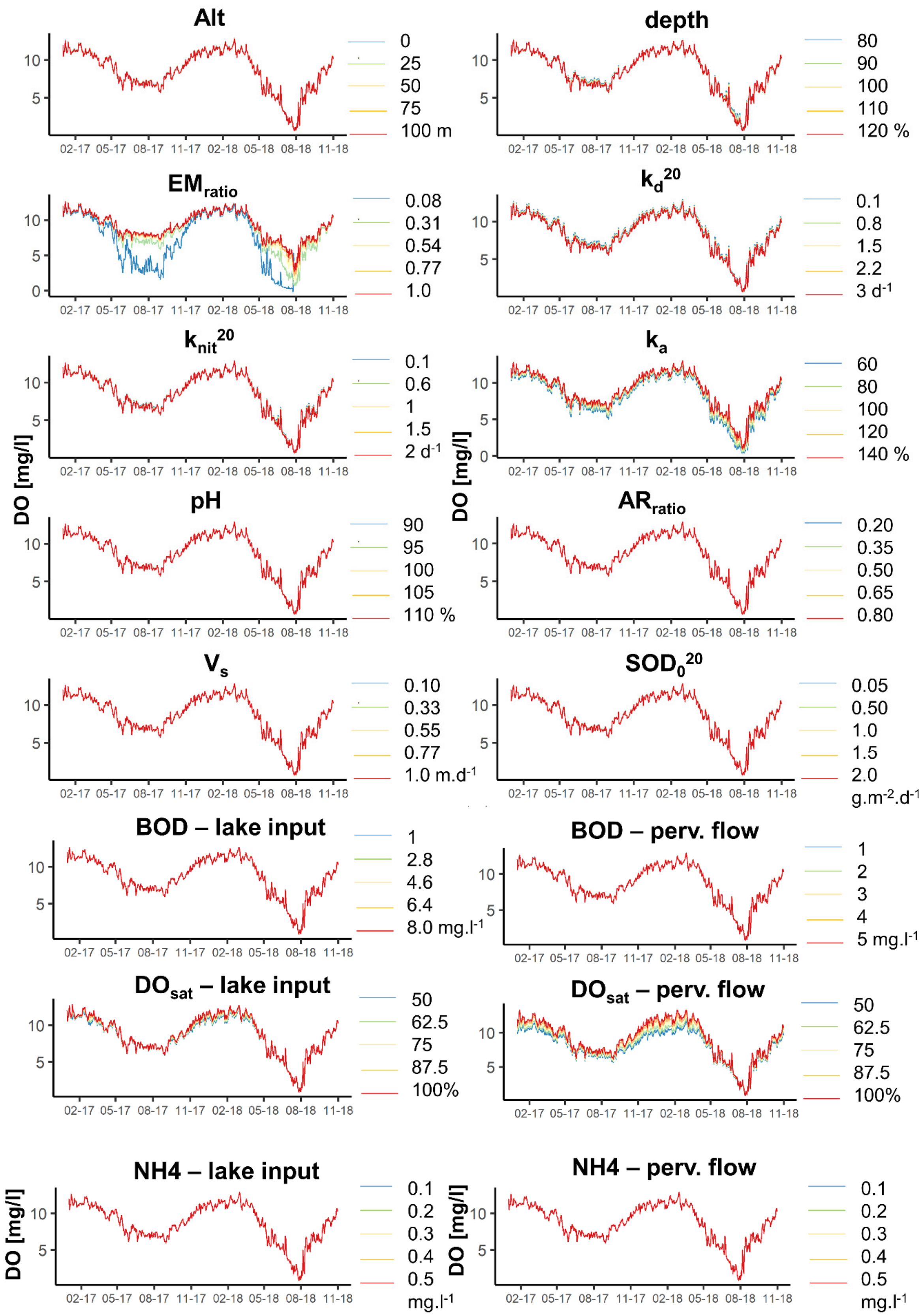


Figure S18. Sensitivity testing for the DO concentration simulation (Parallelvej Station). Results are presented at a daily average time-step. Parameters range and references are given in the Table X2 below.

Table X2. Parameter ranges for the sensitivity test related to DO concentration simulations

Parameter	Unit	Description	Range	Reference for range
Alt	m	Field capacity equivalent	[0–100]	GIS data
depth	m	Stream water depth	[80–120%]*	Perturbation of calculation results
EM_{ratio}	-	Ecosystem metabolism ratio	[0.01–1]	Marcarelli et al. (2011) [10–90] percentile
k_d^{20}	day^{-1}	Reference degradation rate constant for organic matter (20 °C)	[0.1–3]	Chapra (1997)
k_{nit}^{20}	day^{-1}	Reference nitrification rate constant (20 °C)	[0.1–2]	Chapra (1997)
k_a	day^{-1}	Reaeration rate constant	[60–140%]	Perturbation of calculation results, based on Palumbo & Brown (2014)
pH	-		[90–110%]*	Perturbation of input data
AR_{ratio}	-	autotrophic respiration ratio	[0.2–0.8]	Hall & Beaulieu (2013)
$V_{s,BOD}$	$m.\,day^{-1}$	Settling velocity, organic matter	[0.1–1]	Chapra (1997)
SOD_o^{20}	$g.\,m^{-2}.\,day^{-1}$	reference Sediment Oxygen Demand (20 °C)	[0.05–2]	Chapra (1997)
BOD (Lake)	$mg.\,l^{-1}$	cBOD from lake inflow	[1–8]	Lemaire (2021)
BOD (perv.inflow)	$mg.\,l^{-1}$	cBOD from pervious flow component	[1–5]	Lemaire (2021)
DO_{sat} (Lake)	%	Sat. level DO from lake	[50–100]	Lemaire (2021)
DO_{sat} (perv.inflow)	%	Sat. level DO from pervious component	[50–100]	estimation
NH_4 (Lake)	$mg.\,l^{-1}$	Ammonium concentration from lake inflow	[0.1–0.5]	Lemaire (2021)
NH_4 (perv. inflow)	$mg.\,l^{-1}$	Ammonium concentration from pervious component	[0.1–0.5]	Lemaire (2021)

*: upper limit bounded by the calibrated model parameters.

Table S1. Summary of available input and monitoring data for the simulated peri-urban catchment. Detailed description and quantitative values can be found in SI (Fig. S2.4, and Table S3). By default, the 6 locations in this table refer to the 6 flow/depth monitoring stations (Sjaelsø, Grønnegade, Ådalsvej, Parallelvej, Nivemølle, Fredtoften, Brønsholmdalsvej ; Fig. 2). (*): Grønnegade, Ådalsvej, Nivemølle station only. The location for pH, temperature and dissolved oxygen monitoring are shown in Fig. 2.

Parameter	Sampling frequency	Location (Fig 2, S2)	Source/References
Land use, elevation	/	Catchment	Danmark Miljøportal (2020)
Sewer network type (extent, imperviousness)	/	Catchment	NOVAFOS (2020)
Air Temperature	Daily	Catchment	Rudersdal et al. (2020)
Precipitation	Hourly	Catchment	DMI (2020b)
Cloud cover	Daily	Outside catchment	DMI (2020a)
Extraterrestrial Radiation	Daily	Catchment	DMI (2020a)
Flow	Hourly	6 locations	Rudersdal et al. (2020)
Water depth	Hourly	6 locations	
Water abstraction	Daily	3 main areas	
Water temperature	Hourly /	1 location	Rudersdal et al. (2020)
	Bi-monthly	3 locations *	Lemaire (2021)
pH	Hourly /	1 location	Rudersdal et al. (2020)
	Bi-monthly	3 locations *	Lemaire (2021)
Oxygen	Hourly	2 locations	Rudersdal et al. (2020)
	Bi-monthly	3 locations *	Lemaire (2021)
Nutrient (NH4+,NO3-,PO¤3-)	Bi-monthly	3 locations *	Lemaire (2021)
Chl-a	Bi-monthly	3 locations *	Lemaire (2021)
CSO flow	Event	Ådalsevej (multiple in reach)	Hørsholm Kommune (2020)
Effluent flow	Daily	3 WWTPs	NOVAFOS (2020)
Effluent properties (temperature, DO sat, Nutrient)	Variable (daily-monthly)	3 WWTPs	NOVAFOS (2020)

Table S2. Overview of the model input data for the Usserød catchment, data type (time series or constant value), associated time range, and source for the baseline simulation. Input data under "Outlet reach 1/Forcing reach 2" are used for the nutrient concentration simulations only (see section "calibration" in the associated manuscript).

Parameter	Unit	Time variable (TV) / Constant (CSTE)	Value or time range	Reference
General input				
Precipitation		Time series	2017-2019, daily	DMI, (2020b)
Air temperature		Time series	2017-2019, daily	DMI (2020a)
Extraterrestrial radiation		Time series	Calculated	Bojanowski (2013)
Lake				
Flow		Time series	2017-2019, daily	Rudersdal et al. (2020)
DO sat		CSTE	0.7	Calibrated
NH3-N		CSTE	0.23	Lemaire (2021)
NO3-N		CSTE	0.2	Lemaire (2021)
BOD		CSTE	4.5	Lemaire (2021)
chl-a		CSTE	0.03	Lemaire (2021)
PO4-P		CSTE	0.12	Lemaire (2021)
Temperature		not available		
Outlet reach 1/Forcing reach 2				
Flow		Time series	2017-2019, daily	Rudersdal et al. (2020)
DO sat		Time series	Nov 18-Oct 19*	Lemaire (2021)
NH3-N		Time series	Nov 18-Oct 19*	Lemaire (2021)
NO3-N		Time series	Nov 18-Oct 19*	Lemaire (2021)
BOD		Time series	Nov 18-Oct 19*	Lemaire (2021)
chl-a		Time series	Nov 18-Oct 19*	Lemaire (2021)
PO4-P		Time series	Nov 18-Oct 19*	Lemaire (2021)
Temperature		Time series	2017-2019, daily	Rudersdal et al. (2020)
pH		Time series	2017-2019, daily	Rudersdal et al. (2020)
Flow component-pervious areas				
Flow		Time series	Calculated	
DO sat		CSTE	0.7	Calibrated
NH3-N		CSTE	0.12	Lemaire (2021)
NO3-N		CSTE	1.7	Lemaire (2021)
BOD		CSTE	2.7	Lemaire (2021)
chl-a		CSTE	0.004	Lemaire (2021)
PO4-P		CSTE	0.07	Lemaire (2021)
Temperature		Time series	Calculated	regression model, SI Fig S6
Tributary				
Flow		Time series	Calculated	
DO sat		CSTE	0.7	Calibrated
NH3-N		CSTE	0.07	Lemaire (2021)
NO3-N		CSTE	1.5	Lemaire (2021)
BOD		CSTE	2.7	Lemaire (2021)
chl-a		CSTE	0.004	Lemaire (2021)
PO4-P		CSTE	0.04	Lemaire (2021)
Temperature		Time series	Calculated	regression model, SI Fig S6
Separated systems				
Flow		Time series	Calculated	
DO sat		CSTE	0.7	Calibrated
NH3-N		CSTE	0.5	25% total-N concentration Danish EPA (2006)
NO3-N		CSTE	0.5	25% total-N concentration Danish EPA (2006)
BOD		CSTE	10	assumption
chl-a		CSTE	0	assumption
PO4-P		CSTE	0.25	50% total-P concentration Danish EPA (2006)
Temperature		Time series	Calculated	regression model, SI Fig S6

Combined Sewer Overflow			
Flow	Time series	Calculated	
DO sat	CSTE	0.7	Calibrated
NH3-N	CSTE	30	mean from daily time serie - inlet WWTP reach 2 (2019) NOVAFOS (2020)
NO3-N	CSTE	1	mean from daily time serie - inlet WWTP reach 2 (2019) NOVAFOS (2020)
BOD	CSTE	230	mean from bi-monthly sampling - inlet WWTP reach 2 (2019) NOVAFOS (2020)
chla	CSTE	0	assumption
PO4-P	CSTE	4	mean from daily time serie - inlet WWTP reach 2 (2019) NOVAFOS (2020)
Temperature	Time series	Calculated	regression model, Fig S6
WWTP (reach Grønnegade)			
Flow	Time series	Calculated	
DO sat	Time series	2017-2019**	NOVAFOS (2020)
NH3-N	Time series	2017-2019**	NOVAFOS (2020)
NO3-N	Time series	2017-2019**	NOVAFOS (2020)
BOD	Time series	3.1	mean monthly sampling (2019) NOVAFOS (2020)
chl-a	CSTE	0	Assumption
PO4-P	Time series	Time serie	50% total-P concentration NOVAFOS (2020)
WWTP (reach Ådalsvej)			
Flow	Time series	2017-2019, daily	NOVAFOS (2020)
DO sat	Time series	2017-2019, daily	NOVAFOS (2020)
NH3-N	Time series	2017-2019, daily	NOVAFOS (2020)
NO3-N	Time series	2017-2019, daily	NOVAFOS (2020)
BOD	CSTE	/	mean bi-monthly sampling (2019) NOVAFOS (2020)
chl-a	0	/	Assumption
PO4-P	Time series	2017-2019, daily	NOVAFOS (2020)
Temperature	Time series	2017-2019, daily	NOVAFOS (2020)

*: Measurement frequency ca. every 6 weeks (n= 10)

**: Uneven measurement frequency ca. every 3 to 5 days

Table S3. Model performance rating for Nash-Sutcliffe Efficiency (NSE), Percent BIAS (PBIAS) and RMSE-observations standard deviation ratio (RSR) according to (Pérez-Sánchez et al., 2017).

Performance	**NSE**	**RSR**	**PBIAS**
Very good	[0.75-1]	[0-0.5]	<+/- 10
Good	[0.65-0.75]	[0.5-0.6]	[+/- 10 - +/-15]
Satisfactory	[0.5-0.65]	[0.6-0.7]	[+/- 15 - +/-25]
Unsatisfactory	<0.5	>0.70	>+/- 25

Where:

$$NSE = 1 - \frac{\sum_{t=1}^{n}(Y_{sim,t} - Y_{meas,t})^2}{\sum_{t=1}^{n}\left(Y_{sim,t} - \overline{Y}_{meas}\right)^2}$$

$$PBIAS = 100 \times \frac{\sum_{t=1}^{n}(Y_{meas,t} - Y_{sim,t})}{\sum_{t=1}^{n} Y_{meas,t}}$$

$$RMSE = \sqrt{\frac{\sum_{t=1}^{n}(Y_{meas,t} - Y_{sim,t})^2}{n}}$$

$$RSR = \frac{RMSE}{STDEV_{obs}} = \sqrt{\frac{\sum_{t=1}^{n}(Y_{meas,t} - Y_{sim,t})^2}{\sum_{t=1}^{n}\left(Y_{meas,t} - \overline{Y}_{meas,t}\right)^2}}$$

$$R^2 = 1 - \frac{\sum_{t=1}^{n}(Y_{meas,t} - \widehat{Y}_{,t})^2}{\sum_{t=1}^{n}(Y_{meas,t} - \overline{Y}_{meas})^2}$$

Table S4. Model parameters, all reaches (A: Grønnegade, B: Ådalsvej, C: Parallelvej, D: Nivemølle, E: Fredtoften, F: Brønsholmdalsvej (compare Fig. 2). If not explicitly given, the parameter value is uniform across all reaches and "/" indicates this parameter is not relevant in a given reach. Parameter descriptions are given in Appendix A.

Parameter	A	B	C	D	E	F	Reference
Catchment and reach characteristics							
Alt $[m]$							8, from DSFE (2020)
A $[km^2]$	2.08	11.65	1.30	3.90	15.5	18.5	DSFE (2020)
L $[m]$	1600	3000	1900	3550	4200	6100	DSFE (2020)
b $[m]$	3	2.75	3.25	3.25	1.25	1.25	DSFE (2020)
s [‰]	1.1	3.0	1.5	1.5	1.5	1.5	Rudersdal (2018)
f_{imp} [-]	0.03	0.2	0.25	0.28	0	0.05	NOVAFOS (2020)
f_{cs} [-]	0.5	0.65	0.5	0.1	-	0	NOVAFOS (2020)
f_{ss} [-]	0.5	0.35	0.5	0.9	-	1	NOVAFOS (2020)
Hydrological model parameters							
FC $[mm]$							140 (Calibrated)
LP $[mm]$							50 (Calibrated)
β [-]							4 (Calibrated)
SMT $[mm]$							55 (Calibrated)
RTC $[day]$							0.125 (Calibrated)
$UITC$ $[day]$							0.035 (Calibrated)
$LITC$ $[day]$							0.005 (Calibrated)
$PRTC$ $[day]$							0.009 (Calibrated)
$DSMT$ $[day]$							0.002 (Calibrated)
SDR $[day]$							0.5 (Calibrated)
GW $[mm]$ (t=0)	2000	100	1000	1000	0	2000	(Calibrated)
$Contrib_{GWAR}$ $[-]$							0.01 (assumption)
GSI [-]	0	0	-3e-4	-3e-4	0	0	Calibrated
$SSTC$ $[day]$	/	0.05	/	/	/	/	Calibrated
$CSTC$ $[day]$	/	0.5	/	/	/	/	Calibrated
$CSOTC$ $[day]$	/	0.95	/	/	/	/	Calibrated
$\overline{Q_{dry}}$ $[m^3.day^{-1}]$	/	5700	/	/	/	/	Calibrated
Q_{MAX} $[m^3.day^{-1}]$	/	50000	/	/	/	/	Calibrated
$V_{threshold}$ $[m^3]$	/	10000	/	/	/	/	Calibrated
Temperature							
Ρ $[kg/\,m^3]$							1000
Cp $[kg/\,m^3]$							4182
K $[J/(m^2.°C.kg.day)]$							1.9e[6] Bogan et al. (2003)
Oxygen and nutrients							
θ_a $[-]$							1.024, from Chapra (1997)
k_d^{20} $[day^{-1}]$							0.5, from Chapra (1997)
θ_{BOD} $[-]$							1.047, from Bowie et al. (1985)
$V_{s,BOD}$ $[m.day^{-1}]$							0.1, from Chapra (1997)
r_{on} $[g.gN^{-1}]$							4.57, from Chapra (1997)
k_{nit}^{20} $[day^{-1}]$							0.3, from Bowie et al. (1985)
θ_{nit} $[-]$							1.085, from Bowie et al. (1985)
k_{denit}^{20} $[day^{-1}]$							0.1, from Bowie et al. (1985)
θ_{denit} $[-]$							1.045, from Bowie et al. (1985)
$k_{s,denit\_lim}$ $[mg.l^{-1}]$							0.1, from Bowie et al. (1985)
SOD_o^{20} $[g.m^{-2}.day^{-1}]$							1, from Bowie et al. (1985)
θ_{SOD} $[-]$							1.065, from Bowie et al. (1985)
k_{s,o_lim} $[mg.l^{-1}]$							1.4, from Bowie et al. (1985)
Freshwater plant and algae biomass							
$V_{set,sus}$ $[m.day^{-1}]$							0.1, from Bowie et al. (1985)
$G_{max,sus}$ $[day^{-1}]$							2, from Bowie et al. (1985)

$G_{max,mac}[day^{-1}]$	0.1, from Nielsen & Sand-Jensen (1991)
$k_{s,P\_lim}[mgP.l^{-1}]$	0.025, from Bowie et al. (1985)
k_{s,N_lim} $[mgN.l^{-1}]$	0.0005, from Bowie et al. (1985)
$\gamma_{l,background}$ $[m^{-1}]$	0.5, from Julian et al. (2008)
γ_{l,bio_sus} $[m^{-1}.l.mgchla^{-1}]$	0.035, from Chapra (1997)
I_{opt} $[ly.day^{-1}]$	200, from Bowie et al. (1985)
$\emptyset_{atm}$ $[-]$	0.38, from Wild et al. (2019)
$\emptyset_{PAR}[-]$	0.47, from Carr et al. (1997)
$\emptyset_{reflec}$ $[-]$	0.1, from Julian et al. (2008)
r_{oa} $[mg.\mu gChla^{-1}]$	1.5 (calibrated)
AR_{ratio} $[-]$	0.45, from Hall & Beaulieu (2013)
EM_{ratio} $[-]$	0.26 (Calibrated)

Table S5. Parameter probability distributions used for the MC simulation for dissolved oxygen concentration shown in Fig. 6.

State variable	Parameter	Value or time range	Source
DO			
	Saturation DO init. lake inflow	[DOsat]~U[50,100] %	Lemaire (2021)
	Saturation DO init. – nat. flow component	[DOsat]~U[60,100] %	Estimate
	Saturation DO init. - separated systems	[DOsat]~U[60,100] %	Estimate
	Saturation DO init. - CSOs	[DOsat]~U[30,100] %	Estimate
	Reach DOsat estimate	Perturbation calculated value U[-10,+10]%	Estimate
	Reaeration rate	Perturbation calculated value $k_a.U$[-40,+40]%	Palumbo & Brown (2014)
	Ecosystem metabolism ratio	$EM_{ratio} \sim U$[0.01-1]	Marcarelli et al. (2011)
	Autotrophic respiration ratio	$AR_{ratio} \sim U$[0.3,0.7]	Estimate
	BOD concentration (WWTP reach C)	$BOD \sim logN$[2.5,5] $mg.l^{-1}$	(NOVAFOS (2020)
	BOD degradation rate	$k_d \sim U$[0.1,0.3] day^{-1}	Chapra (1997)
	SOD background	$SOD_{BG} \sim U$[0.1,2] $g.m^2.day^{-1}$	Chapra (1997)
	Optimal growth macrophyte	$G_{max} \sim U$[0.01,0.2] day^{-1}	(Nielsen & Sand-Jensen, 1991)
	Optimal light level	$I_{opt} \sim U$[100,300] $ly.day^{-1}$	Bowie et al. (1985)
	Nitrification rate	$k_{nit}^{20} \sim U$[0.2, 6] day^{-1}	Bowie et al. (1985)
	Attenuation cloud cover	Perturbation calculated value $\emptyset_{cloud}.U$[-40,+40]%	Estimate
	Oxygen yield per unit biomass	$r_{oa} \sim U$[0.5,2.5] $mg.\mu gChla^{-1}$	Krause-Jensen & Sand-Jensen (1998)

Table S6. Parameter probability distributions used for setting up the MC simulation regarding physico-chemical conditions and shown in Fig. 7.

State variable	Parameter	Distribution	Reference
Stream temperature			
	Natural flow component temperature	Perturbation regression baseline parameters: U[-10,+10]%	Estimate, Fig S6.
	Equilibrium temperature	Perturbation regression baseline parameters: U[-10,+10]%	Estimate, Appendix A
	Coefficient heat transfer	$K \sim U$[1.9e6, 2.4e6]	Bogan et al. (2003)
Inorganic nitrogen (NH4-N, NO3-N)			
	NH4 concentration nat. flow component	[NH4-N]~N[0.12,0.13] mg-N/l	Thodsen et al. (2016)
	NO3 concentration nat. flow component	[NO3-N]~N[3.16,2.07] mg-N/l	Thodsen et al. (2016)
	NH4 concentration - Separated systems	Perturbation baseline value U[-50,+50]%	Estimate, Table S1
	NO3 concentration - Separated systems	Perturbation baseline value U[-50,+50]%	Estimate, Table S1
	NH4 concentration - CSOs	Perturbation baseline value U[-50,+50]%	Estimate, Table S1
	NO3 concentration -CSOs	Perturbation baseline value U[-50,+50]%	Estimate, Table S1
	Nitrification rate	$k_{nit}^{20} \sim U$[0.2, 6] day^{-1}	Bowie et al. (1985)
	Denitrification rate k_{denit}	$k_{denit}^{20} \sim U$[0.1, 1] day^{-1}	Bowie et al. (1985)
Dissolved reactive Phosphorus (PO4-P)			
	PO4 concentration nat. flow component	[PO4-P]~N[0.06,0.07] mg-P/l	Thodsen et al. (2016)
	PO4 concentration -Tributary	Perturbation baseline value U[-50,+50]%	Estimate, Table S1
	PO4 concentration -Separated systems	Perturbation baseline value U[-50,+50]%	Estimate, Table S1
	PO4 concentration - CSOs	Perturbation baseline value U[-50,+50]%	Estimate, Table S1
	PO4 concentration - WWTP	Perturbation baseline value U[-50,+50]%	Estimate, Table S1
Suspended chl-a			
	Optimum growth rate	$G_{max,sus} \sim U$[0.2-3] day^{-1}	Bowie et al. (1985)
	Maintenance/respiration/loss rate	$k_r^{20} \sim U$[-50,+50]%. $G_{max,sus}$	Bowie et al. (1985)
	Temperature optimal growth	$T_{opt} \sim U[15-30]°C$	Bowie et al. (1985)
	Light Attenuation coefficient biomass	Perturbation default value γ_{l,bio_sus}. U[-30,+30]%	Estimate, Appendix A
	Settling velocity	$V_{set,sus} \sim U[0.01-1] m.day^{-1}$	Chapra (1997)

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