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Evaluation of a coupled hydrodynamic-closed ecological cycle approach for modelling dissolved oxygen in surface waters

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Abstract

The description of intertwined ecological processes in surface waters requires a holistic approach that accounts for spatially distributed hydrological/water quality processes. This study describes a new approach to model dissolved oxygen (DO) based on linked hydrodynamic and closed nutrient cycle ecological models. Long term datasets from the River Dommel (Netherlands) are used to determine: 1) if this methodology is suitable for modelling DO concentrations, 2) the model sensitivity to various levels of nutrients input, and 3) the DO production and consumption processes and their response to nutrient input changes. Results show that seasonal dynamics of DO are well quantified at long timescales; the sensitivity of DO to different pollutant sources exhibits significant seasonal variation and the largest influences on DO are aeration and mineralization of organic material. The approach demonstrates an ability to consider the impacts of nutrient input and long term vegetation maintenance on ecological quality.

Software Requirements

- Wageningen Lowland Runoff Simulator (WALRUS) developed by Brauer et al. (2014) available through the following website https://github.com/ClaudiaBrauer/WALRUS
- SOBEK River one-dimensional (1D) and D-Water Quality module delivered by Deltares Software Center
- PCDitch is available through STOWA (Acronym for Foundation for Applied Water Research). More information on PCDitch and PCLake can be found at: https://www.stowa.nl/onderwerpen/waterkwaliteit/realiseren-van-ecologische-waterkwaliteitsdoelen-krw/pclake-en-pcditch
- MATLAB for data analysis of PCDitch results, Jupyter Notebook and ARCGIS for data results presentation, R-Studio for model implementation and parameter optimization of WALRUS model

1 Introduction

The European Union (EU) Water Framework Directive (WFD) requires that a ‘good ecological status’ should be achieved and maintained in all surface water and groundwater (Council of European Commission, 2000). A good ecological status is established by the biological, chemical and hydrological characteristics of the water body. Moreover, EU member states have specific interpretations of what is considered ‘good ecological status’. For example, in the Netherlands key ecological factors and water system analyses are used as a method to understand ecological water quality processes and to define goals and measures for water bodies. These key ecological factors cover a ‘crossing’ between human pressures on a water body (e.g. channelization, vegetation maintenance or diffuse pollution) and environmental factors (e.g. temperature regime, substrate variation or nutrient concentration) (STOWA, 2015). Water quality modelling can be used at different spatial and temporal scales to understand relationships between human pressures on a water body and environmental factors as well as enabling discussions amongst stakeholders of potential intervention, management or maintenance strategies. As catchments are complex systems encompassing a vast quantity of processes and components, integrated water quality modelling is currently the preferred choice (Tscheikner-Gratl et al., 2018) for determining the best management practices to address both urban and rural pressures for the improvement of the water body.

Modelling river water quality has generally been conducted using the advection-dispersion-reactions approach (which may also include terms for transient storage, biota uptake, groundwater and lateral flows, sediment deposition or uptake). The advection and dispersion processes are usually described within the hydrological/hydrodynamic model and the biochemical and physical conversion processes are described within reactions equations (Rauch et al., 1998). Most surface water quality studies have focused separately on these processes and over various time scales. For instance, solute transport using advection-dispersion equations with point source pollution have been widely applied in river systems (Ani et al., 2009; van Mazijk and Veling, 2005; Wallis et al., 2014) More detailed modelling approaches including the effects of transient storage and hyporheic exchange have also been developed such as the Transient Storage Model (Ge and Boufadel, 2006; Runkel, 1998). Dissolved oxygen and biochemical models represent the dynamics of reaeration and decomposition of organic matter (Streeter et al., 1925). Important additional oxygen production and consumption processes such as the removal of Biological Oxygen Demand (Dobbins, 1964), oxygen production and uptake due to periphyton biomass (Welch et al., 1989) and the dynamics of nutrient cycling and algae have been incorporated in other water quality models such as the QUAL2 family of models (Brown, 1987) and the River Water Quality Model no. 1 (Reichert et al., 2001). Moreover, eutrophication models in varying degrees of complexity (e.g. modelling nutrient enrichment due to various processes) can be used over longer time scales to study interactions between macrophytes, phytoplankton and nutrients in the ecosystem. However, to date eutrophication models have been primarily applied to lake systems or to study the nutrient transport to the destination ecosystems such as estuaries or oceans (Nijboer and Verdonschot, 2004).

To obtain a complete physical, chemical and ecological description of the river catchment for ecological status evaluation, integrated modelling approaches covering both urban and rural catchments, have gained popularity over the past years (Holguin-Gonzalez et al., 2013; Mouton et al., 2009). Mouton et al. (2009) used the Water Framework Directive (WFD)-Explorer Toolbox to evaluate the ecological status of the Zwalm River in Belgium. Their study integrated a hydraulic model, with a mass balance module to assess ecological pressures based on expert knowledge. However, the approach oversimplified water quality processes, and had a coarse catchment scale (Holguin-Gonzalez et al., 2013). Holguin-Gonzalez et al. (2013) developed a framework integrating a MIKE 11 hydraulic and physicochemical water quality model with two ecological models based on habitat suitability and ecological assessment with an emphasis on macroinvertebrates. However, the QUAL2E and MIKE11 models lack the ability to represent sediment processes as biological conversions. This disables their capability to model closed nutrient cycles (Trinh Anh et al., 2006) which is beneficial to account for the nutrient ratios at the various trophic levels.

A holistic ‘combined modelling approach’ incorporating the long term intertwined dynamics of flow, nutrients and aquatic biota and physical and ecological interactions is still lacking in the literature. More specifically, the capability to model closed nutrient cycles, plant competition, organisms, water and sediment processes using an extensive ecological model coupled to a hydrologic and hydrodynamic model is still pending. Therefore, in this study, we adopt such ‘combined modelling approach’ to represent the medium to long-term hydrological processes of a catchment (precipitation, evapotranspiration and runoff), transport and mixing processes from both urban (pollution loadings of CSOs and WWTP) and rural areas, and ecological processes in a slow flowing river system. This combined approach is illustrated in Figure 1 where the three main rainfall-runoff, hydrodynamic and ecological models are shown with their corresponding data requirements. The main objectives of the study are: 1) to evaluate the capability of the combined modelling approach to simulate DO for medium to long term time scales (months to years), 2) to determine the sensitivity of DO model predictions a in the river system given uncertainty in the input boundary conditions, and 3) to determine the dominant oxygen production and consumption processes and their sensitivity to the changes in input boundary conditions. The novelty of this study is the combination of a hydrodynamic and ecological model which include urban and rural components and their interactions within the ecological closed nutrients cycles. This can also include the effects of river management practices such as vegetation clearance and dredging. In addition, this methodology can include the effects of nutrient inputs and cycling from rural areas, Combined Sewer Overflows (CSOs) and a Wastewater Treatment Plant (WWTP) on oxygen, nutrient and biota concentrations in the river system. Inclusion of both rural and urban inputs has been recognized as the ideal modelling approach. However, to date, few studies have successfully implemented such methodology (Honti et al., 2017; Tscheikner-Gratl et al., 2018).

The nutrient and vegetation model for ditches PCDitch was used in this study. Originally developed for lakes (PCLake), PCDitch was selected because it is among the most extensive ecosystem models to date which can include the competition for nutrients, light and temperature and can model production by plants, algae, reaeration and oxygen consumption due to different water and sediment processes (Janse, 2005; Trolle et al., 2014). In addition, PCDitch is a dynamic model that describes the dominant biological components in the river using closed nutrient cycles. The closed mass balance approach is implemented through nutrient-to-dry weight ratios. This allows the stoichiometry of organisms to change with trophic level (Mooij et al., 2010). Management practices such as mowing and dredging can also be implemented in PCDitch allowing water managers to identify target measures on specific processes that assist to improve the quality of the river system. However, the capability of PCDitch to simulate ecological conditions in rivers has not been tested, neither has its capability to predict changes in dissolved oxygen (DO) concentration as a by-product of the various biochemical and ecological processes (e.g. mineralization of organic material, respiration and production of macrophytes). For this to be attempted, coupling with rainfall runoff and hydrodynamic models is required.

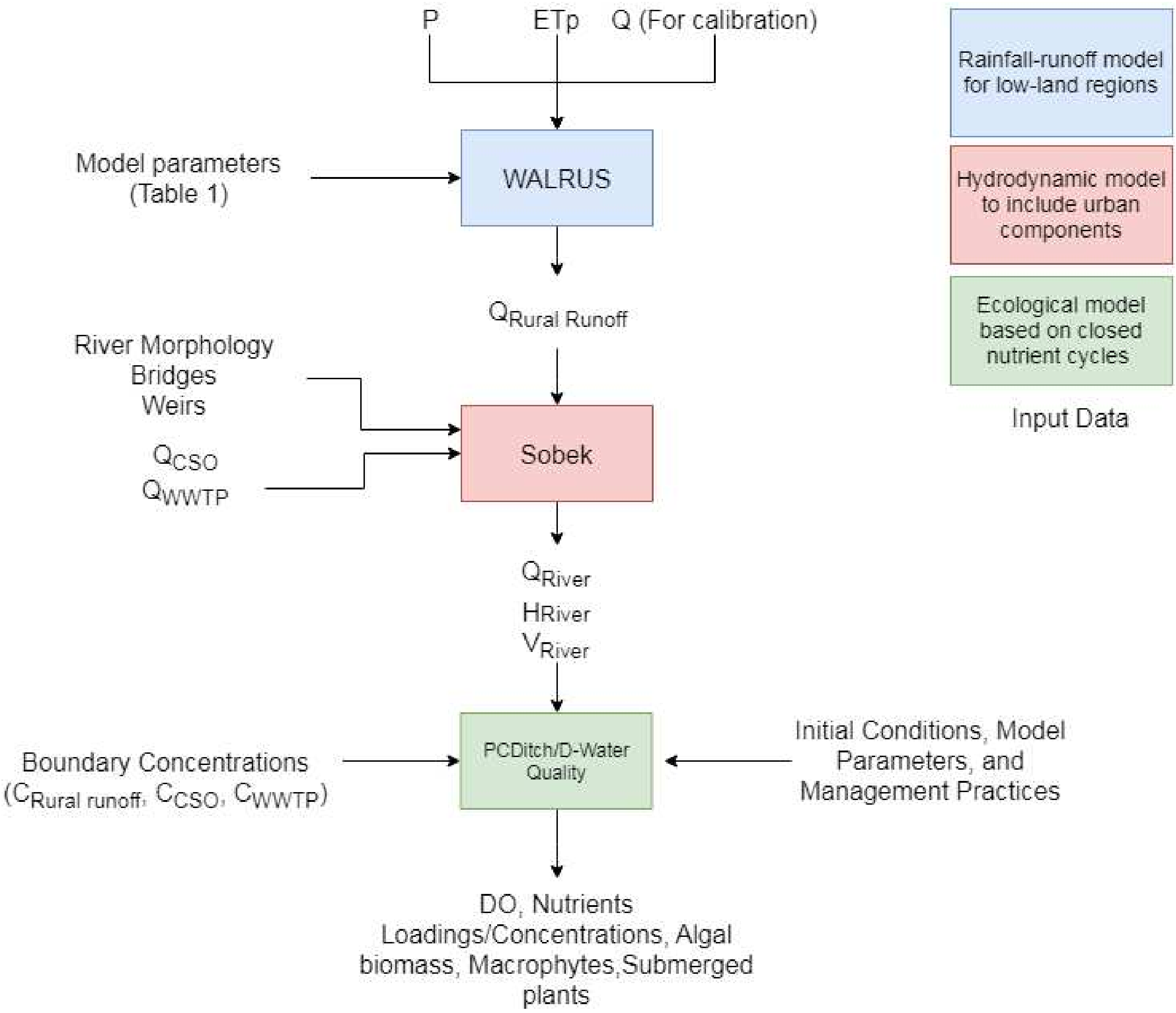

Figure 1. Combined modelling diagram. WALRUS model inputs: precipitation (P), potential evapotranspiration (ETp), river discharge (Q), and model parameters used in calculation of surface and groundwater runoff ($Q_{Rural\ Runoff}$). Sobek inputs: Combined Sewer Overflows discharge (Q_{CSO}), Wastewater Treatment Plant Discharge (Q_{WWTP}), river morphology, and river structures used in calculation of total river discharge (Q_{river}), depth (H_{river}), and velocity (V_{river}). PCDitcht/D-Water Quality inputs: Input boundary concentrations for the rural runoff ($C_{Rural\ Runoff}$), Combined Sewer Overflows (C_{CSO}), and Wastewater Treatment Plant (C_{WWTP}) to calculate DO and ecological variables.

2 Methodology

2.1 Study Area Description

The Dommel River (shown in Figure 2) flows from the northeast of Belgium to the south of the Netherlands until it joins the Meuse River. The upstream region of the catchment is heavily influenced by agriculture, mainly livestock farming, while the downstream area runs through the city of Eindhoven (Netherlands). The river receives urban discharges from approximately 750,000 P.E. (population equivalent) from the Eindhoven WWTP and over 200 CSOs (Weijers et al., 2012). In the summer, the WWTP discharge on the river can account for up to 50% of the Dommel baseflow of 1.5 m^3s^{-1} (Langeveld et al., 2013b). The geology is dominated by sandy deposits with small amounts of mica, feldspars and clay minerals (Petelet-Giraud et al., 2009). Pollution sources include nitrogen and phosphates leaching from agriculture (mainly manure application) and urban inputs from CSOs and WWTP discharges. Figure 2 shows the main flow contributions to the Dommel River and the locations where measured daily flow, dissolved oxygen, total nitrogen, and total phosphorus concentrations are available. The flow contributions include surface and groundwater runoff sources which for simplicity in this paper are referred as ‘runoff’, CSOs and the Eindhoven wastewater treatment plant (WWTP). These sources are described in more detail in section 3.4.1

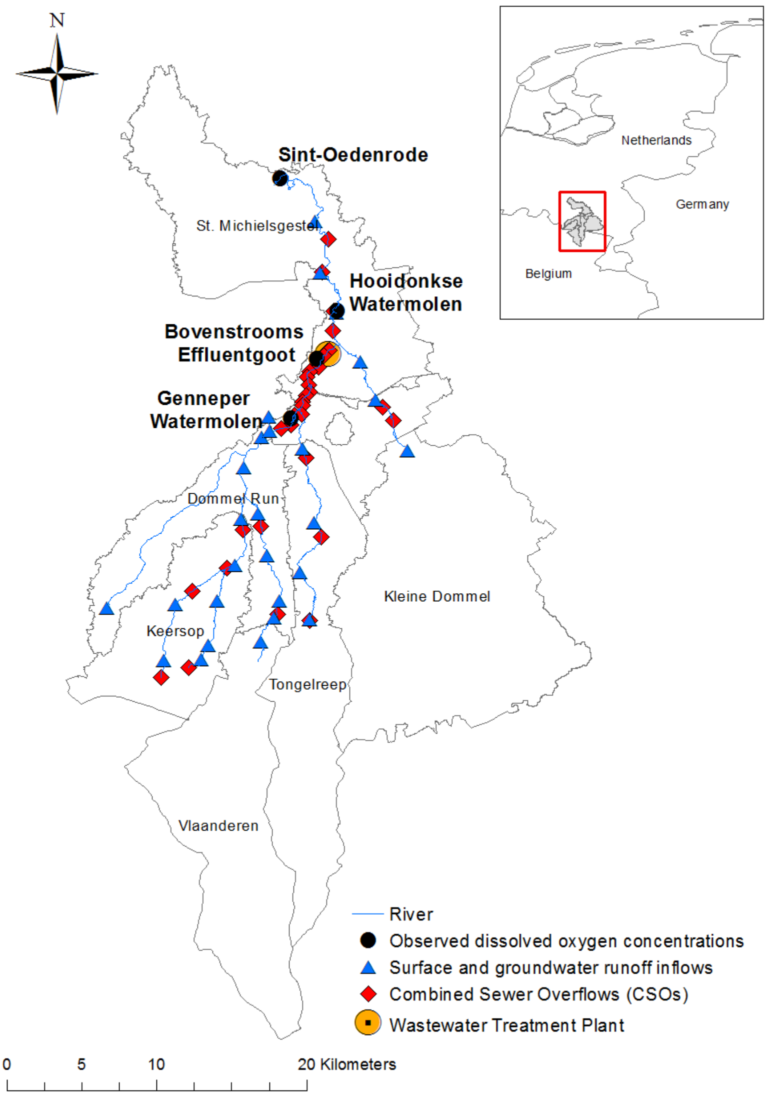

Figure 2. Model schematization and subcatchments of the Dommel River catchment

2.2 Rainfall-Runoff Modelling

The study area was divided into six sub catchments (Figure 2). A rainfall-runoff model was created for each sub catchment using the Wageningen Lowland Runoff Simulator (WALRUS) model. WALRUS is a water balance model which considers various reservoirs (groundwater, vadose zone, and surface water) and fluxes between the reservoirs (Brauer et al., 2014). Precipitation can be transferred to the surface water reservoir directly, infiltrate into the vadose zone, or travel to the surface water reservoir via quickflow. A quickflow reservoir is used to represent the accumulation of overland, macropore and drainpipe flow. The water level at the surface water reservoir with respect to time is found using the following equation presented in Brauer et al. (2014):

$$\frac{dh_S}{dt} = \frac{f_{XS} + P_S - ET_S + f_{GS} + f_{QS} - Q_S}{a_S}$$

Where f_{XS} is the surface water supply/extraction in (mmhr-1), P_S is the precipitation into surface water reservoir (mmhr-1), ET_S is the potential evapotranspiration (mmhr-1), f_{GS} is the groundwater drainage/surface water infiltration (mmhr-1), f_{QS} is the inflow from the quickflow reservoir (mmhr-1), Q_S is the stage–discharge relationship (mmhr-1), and a_S is the surface water area fraction (-). Discharge is calculated by the Manning's stage-discharge relationship (Manning et al., 1890).

WALRUS was selected because of its ability to account for dominant low-land areas processes such as couplings between the groundwater and unsaturated zone, flow routes that depend on wetness conditions, and interactions between groundwater and surface water (Brauer et al., 2014).

The WALRUS model inputs include precipitation and evapotranspiration data. Measured discharge data was used for model calibration. Data was collected from January 1st, 2011 to December 31st, 2013. Hourly precipitation rates were obtained from merged radar and rain gauge data from the Dutch meteorological agency (KNMI) and the Dommel Water Board (Moreno-Ródenas et al., 2017). Daily Penman-Monteith evapotranspiration rates were obtained from the Foundation for Applied Water Research (Stichting Toegepast Onderzoek Waterbeheer) in the Netherlands (STOWA, 2013). Hourly discharge was available for the Keersop, Tongelreep and St. Michielsgestel sub catchments from the Dommel Water Board. The total observed runoff from the Keersop and Tongelreep catchments were separated into its rural and urban runoff components using the sub-flow separation technique suggested by Willems (2009) to account for contributing flows from combined sewer overflows (CSOs). The flow at Sint-Oedenrode (from the St. Michielsgestel sub catchment) was not subdivided into sub flows due to the large contribution of the wastewater treatment plant discharge. Therefore, this sub catchment was not used for calibration of the rainfall-runoff model. The Keersop and Tongelreep sub catchments were used to calibrate the model parameters (Table 1), which was then also applied to the other sub catchments. This calibration was carried out using the swarm optimization technique hydroPSO available in the WALRUS model. The parameters in Table 1 remained constant for the studied catchments including groundwater depths, surface water fractions, quickflow and groundwater reservoir constants and soil properties.

Table 1. WALRUS Model parameters per sub catchment

Parameter	Unit	Abbreviation	Value
Surface water parameter bankfull discharge	(mm h^{-1})	cS	4.0
Initial groundwater depth	(mm)	dG0	1200
Channel depth	(mm)	cD	2750-3250
Surface water area fraction	(-)	aS	0.0090
Soil type	(-)	st	loamy sand
Wetness index parameter	(mm)	cW	400
Vadose zone relation time	(h)	cV	4

Groundwater reservoir constant	(mm h)	cG	30,000,000
Quickflow reservoir constant	(h)	cQ	25

2.3 Hydrodynamic Modelling

A SOBEK-River one-dimensional (1D) model was provided by the Dommel Water Board containing the river network shown in Figure 2. SOBEK is based on the 1D Saint Venant equations (dynamic wave) and utilises the Delft numerical scheme (Deltares, 2014). This model was used to estimate the spatially distributed hydraulic characteristics of the river network including flow velocities, volumes and discharges. 6,214 consecutive reaches ranging from 0.04m to 200m in length (with an average of 25m per reach) formed the river network. The model schematization includes 1,696 cross sections, 29 runoff inflows (shown as the Surface and Groundwater Runoff inflows), 2 boundary outflows, 27 lateral flows (shown as the CSOs), 146 weirs and 211 bridges and 2018 Connection Nodes with Storage and Lateral Flow. Culverts were removed from the SOBEK model in order to accelerate the simulation and reduce instabilities, this was deemed acceptable as no flooding or culvert surcharge occurred during the simulated period. The bed friction was represented using Strickler's roughness coefficient Ks ($m^{1/3}s^{-1}$) (Deltares, 2014). The Ks coefficient for the Dommel River was set to 25 $m^{1/3}s^{-1}$ based on previous studies and analysis as conducted by the Dommel Water Board.

The Surface and Groundwater Runoff inflow boundary conditions were implemented in the SOBEK hydrodynamic model from the runoff generated using the WALRUS model. The flows at the outlet of the sub catchments were divided into sub flows according to hydrological areas based on the natural drainage as observed in (Langeveld et al., 2013a). The 27 clusters of CSOs were included in SOBEK to represent the urban inputs as lateral inflows in the river schematization, containing monitored discharge data with a frequency of every 15 minutes for the three years from Jan 1, 2011 to December 31, 2013. Similarly, hourly WWTP discharge was also included as a lateral inflow for the same period. A flow weir located between the Dommel Run and the Sint-Oedenrode subcatchments represented the flow control during summer (1.5 m^3s^{-1}) and winter (0.75 m^3s^{-1}).

2.4 Water Quality Modelling

SOBEK conventionally describes mixing and dispersion processes using the 1D Advection Dispersion Equation (Taylor, 1954), which dispersion coefficient is defined as a linear function of the concentration gradient between the river reaches (Deltares, 2014). However, in this case, the daily temporal resolution of the model resulted in negligible concentration gradients and hence simulations based on the assumption of instantaneous mixing over each reach. The potential implications of this assumption are described further in Section 4.

The model PCDitch was used to simulate the biochemical and ecological components in the river such as dissolved oxygen concentrations, dry organic matter, nutrient concentrations, Secchi depth and biomass coverage. PCDitch is a plant/nutrient based competition model that includes the water column and upper sediment layer incorporating the competition for nutrients from submerged rooted and non-rooted vegetation, floating duckweed, algae, Charophytes, Nymphaeids and Helophytes. Macrophytes groups are limited by light, nutrients and temperature. A more comprehensive description of PCDitch is found in (Janse, 2005).

PCDitch is used in conjunction with the water quality and transport package D-Water Quality (Deltares, 2018). This platform uses the finite volumes method to solve the advection-dispersion-reaction equation. Furthermore, the hydrodynamic information (e.g. the river mean water depths, water inflows and retention times) was still retrieved from SOBEK and processed by D-Water Quality/PCDitch. The simulation was carried out for a period of three years from Jan 1st 2011 to Dec 31st 2013. Hourly monitored temperatures were obtained from the Dommel Water Board and implemented in the model. The effects of in river mowing and dredging were included in the model. Mowing was set to twice per year removing 95% of the vegetation and dredging was set yearly with a removal of 1 cm of the bottom bed thickness.

Sedimentation, settling and resuspension are included in the ecological model. The sediment top layer consisting of particulate matter (organic and inorganic) and pore water (with dissolved nutrients). Settling of small inorganic particles (humus and detritus) is described in the ecological model as a first-order equation where the settling velocity is inversely related to the water depth. The settling of bigger particles (> sand particles) is not included since these generally settle within the time scale of hours, which is shorter than the time resolution of PCDitch. Resuspension is modelled as a zeroth order process. As the settling rate decreases, the resuspension rate increases with the size of the water body. Resuspension is enhanced by sediment porosity, and mitigated by vegetation cover. A process of burial is also included, where a top layer of sediment is added to the net increase of sediment material to maintain a fixed sediment thickness layer and closed nutrient cycle (Janse, 2005).

2.5 Set-up of boundary conditions: Rural runoff, CSOs, WWTP and Connection Nodes

External water quality concentrations were defined in PCDitch for the rural runoff, CSOs, WWTP flow and connection Nodes with Storage and Lateral Flow. Table 2 presents the PCDitch inputs required for each boundary including: the dry weights of detritus (mg DW l^{-1}), inorganic matter and phytoplankton (mg DW l^{-1}), the concentrations of nitrogen in detritus, ammonium, nitrate and phytoplankton (mgN l^{-1}), the concentration of dissolved oxygen (mgO_2 l^{-1}) and the phosphorus concentrations in adsorbed inorganic matter, detritus, phosphate and phytoplankton (mgP l^{-1}). Detritus concentrations were used to describe the total amount of organic matter. Detritus was used because it is the only available parameter in PCDitch to describe organic matter loads. The detritus and inorganic matter concentrations were approximated from the percentage of organic matter (OM) and concentrations of total suspended solids in the water column (TSS). Incoming amounts of phytoplankton were assumed to be negligible from the three external sources since rural runoff, CSO and WWTP outflows usually do not contain phytoplankton, apart from some remnants of biofilm, which are accounted for in the detritus concentrations. The nitrogen and phosphorus amounts in detritus were estimated using the relationships shown in Table 2. Adsorbed phosphorus was estimated as the remainder from subtracting phosphate (PO_4) from total phosphorus (Ptot). Dissolved oxygen (O_2), ammonium (NH_4), nitrate (NO_3) and phosphate (PO_4) concentrations were obtained from collected field measurements by the Water Board. The water quality concentrations from the wastewater treatment plant discharge into the river were simulated. An explanation regarding the WWTP discharge simulation, and the description of the input concentrations for each boundary and how they were obtained is given in the following paragraphs.

Table 2. PCDitch Boundary inputs and their estimation methods. Detritus and inorganic matter are estimated from the Total Suspended Solids (TSS) and Organic Matter percentage (OM). Adsorbed phosphorus is estimated from Total Phosphorus (Ptot)

Parameter	Abbreviation	Units	Estimation method
Detritus in water	*Det*	mgDW l^{-1}	*Physical relation: TSS*OM /100*
Inorganic Matter (IM) in water	*IM*	mgDW l^{-1}	*Physical relation: TSS*(100-OM) /100*
Phytoplankton	*Phyt*	mgDW l^{-1}	*Negligible*
Nitrogen in detritus	*NDet*	mgN l^{-1}	*Standard assumption in PCDitch: Det* 0.025*
Ammonium in water	*NH4*	mgN l^{-1}	*Measured, simulated for WWTP*
Nitrate in water	*NO3*	mgN l^{-1}	*Measured, simulated for WWTP*
Nitrogen in phytoplankton	*NPhyt*	mgN l^{-1}	*Negligible*
Dissolved oxygen in water	*O2*	mgO_2 l^{-1}	*Measured, simulated for WWTP*

Adsorbed phosphorus on IM in water	*PAIM*	mgP l^{-1}	*Physical relation: Ptot - PO4- PDet*
Phosphorus in detritus	*PDet*	mgP l^{-1}	*Standard assumption in PCDitch: Det* 0.0025*
Phosphate in water	*PO4*	mgP l^{-1}	*Measured, simulated for WWTP*
Phosphorus in phytoplankton	*PPhyt*	mgP l^{-1}	*Negligible*

Rural runoff water quality characterization

The rural inflows relate to surface and groundwater runoff from agricultural and natural areas. These flows were quantified using the WALRUS model. The mean concentrations in Table 3 were used for the input boundary conditions. Monthly water quality input concentrations were obtained from monitored data provided by the Dommel Water Board for the years 2011 to 2013. These include total nitrogen (TN), ammonium (NH_4), total phosphorus (TP), phosphate (PO_4), dissolved oxygen (O_2) and total suspended solids (TSS). Nitrate concentrations (NO_3) were estimated as half of the total nitrogen concentrations and Kjeldahl nitrogen (Nkj) as the other half. Nitrite was considered negligible. The organic matter content was estimated by subtracting ammonia (NH_4) from Kjeldahl nitrogen and then dividing it by the total nitrogen concentration.

CSOs water quality characterization

Over 200 CSOs discharge on the Dommel River. Probability distributions for CSO pollutant concentrations were estimated from a monitoring campaign (Moens et al., 2009). The CSO concentrations were added as lateral flows with event mean concentrations. These event mean concentrations have shown to give acceptable model results despite the difficulty in capturing the high variability of CSOs water quality parameters (Moreno-Ródenas et al., 2017).

Wastewater treatment plant water quality characterization

The Dommel receives effluent of the central WWTP in Eindhoven. The Eindhoven WWTP is composed by three biological lines (primary clarifier, activated sludge tanks and secondary clarifiers) with a capacity of 26,000 m^3h^{-1} and a bypass storm settling tank with a capacity of 9,000 m^3h^{-1}. A fully detailed ASM2d bio-kinetic model was created to simulate water quality processes in the WWTP (Benedetti et al., 2013). The influent quantity (sewer network - WWTP) was represented using observed data at the boundary connection. This was derived from three magnetic flow sensors located at three influent pressurised pipes. Influent water quality characteristics were estimated using a calibrated empirical influent generator (Langeveld et al., 2017). Effluent hourly series (Jan 01, 2011 to Dec 31, 2013) were derived from a forward uncertainty propagation scheme accounting for uncertainties in the influent water quality and quantity characteristics. This time series of WWTP water quality discharge were generated to include the dynamics of the treated wastewater quality characteristics during wet and dry weather conditions.

2.5.1 Scenarios for Sensitivity Analysis

To evaluate the effects of the rural runoff, CSOs and WWTP discharge and nutrient inputs on the dissolved oxygen concentrations, three nutrient levels for each of these boundaries were defined as shown in Table 3. The scenarios were selected based on the total phosphorus concentrations. Phosphorus was used as it is an indicator of eutrophication and commonly assumed to be the limiting growth factor for phytoplankton and macrophytes in oligotrophic to mesotrophic waters (Janse, 2005; Newton and Jarell, 1999). Using the observed and simulated data described in section 3.4.1, the three scenarios (Table 3) were defined for each boundary as follows: 1) a 'base' scenario representing average nutrient inputs observed, 2) a 'high' scenario representing higher levels of nutrient inputs, and 3) a 'low' scenario representing lower levels of nutrient inputs. For the rural runoff base scenario, average observed values of total phosphorus concentrations were found with their corresponding water quality parameters (e.g. NO_3, NH_4, O_2, TSS and PO_4). Similarly, for the high and low scenarios, the maximum and minimum observed values of total phosphorus over the period of analysis (2011-2013) were selected with their corresponding datasets of water quality variables. Several datasets presented at Evers and Schipper (2015) were studied at various locations in the catchment to ensure that outliers in the data were not selected. Also, the selected input data was checked against monitored data from the Dommel River Water Board (2019) to ensure that the input concentrations selected were representative of regular water quality concentrations in the river. For the CSOs, the nature of rainfall driven sewer surcharge events results in skewed water quality distributions, with the mean value not providing a good representation of the water quality impacts on the river. Hence the modes of the water quality distributions were used for determining the water quality concentrations of the base scenario with their corresponding water quality parameters, except for the total suspended solids where monitored data was available from (Brouwer, 2012). The 2.5th and 97.5th and percentiles of the CSO frequency distributions were used for determining the high and low nutrient load scenarios. The WWTP scenarios were selected from a total of 99 samples drawn using a Latin Hypercube sampling scheme to describe the variability of the simulated WWTP output. The 2.5th and 97.5th percentiles were used to determine the low and high scenarios for the WWTP based on total phosphorus with their corresponding water quality parameters (Ptot, Kjeldahl Nitrogen, PO_4, NO_2, NH_4, TSS, and NO_3). Given the large quantity of WWTP data generated using the simulation described in Section 2.5, the WWTP low, high and base scenarios are given in Appendix A.

Table 3. High, middle and low scenarios of rural runoff and CSO Water Quality concentrations

Parameter		Rural Runoff Low scenario	Rural Runoff Base scenario	Rural Runoff High scenario	CSOs inflows Low scenario	CSOs inflows Base scenario	CSOs inflows High scenario
PO_4	mg l^{-1}	0.04	0.05	0.08	0.5	0.8	5.7
Ptot	mg l^{-1}	0.1	0.2	0.3	0.5	2.1	34.6
Chl-a	µg l^{-1}	30	35	40	0	0	0
O_2	mg l^{-1}	6.3	6.8	4.4	3.4	4.6	6.2
Ntot	mg l^{-1}	2.8	3.6	4.6	4.5	8.0	16.2
NO_2	mg l^{-1}	0	0	0	0	0	0
NO_3	mg l^{-1}	1.4	1.8	2.3	0.7	1.2	1.7
NH_4	mg l^{-1}	0.1	0.6	1.7	1.6	2.2	4.9
Nkj	mg l^{-1}	1.4	1.8	2.3	3.8	4.8	14.5
TSS	mg l^{-1}	1	15	50	25.0	298	397.0
OM	%	13.0	33.3	48.2	48.9	50.9	59.3

3 Results

The hydrological processes and runoff generation quantified using the WALRUS model for the calibrated catchments can be found in Appendix B. The results of the hydrodynamic simulation (flow versus time) can also be found in the Appendix C. The Nash Sutcliffe Coefficient (NSC) was used to determine the goodness of fit of the hydrodynamic simulation results and the observed flows. According to Moriasi et al. (2007), model performance is satisfactory when NSC is greater than 0.5. The NSC values from this study ranged from 0.5 to 0.7 for the Sint-Oedenrode and Keersop subcatchment outlets, and downstream and upstream locations at the Tongelreep catchment. In the following sections, the results of the integration of the hydrological, hydrodynamic and ecological processes is shown by presenting first the evaluation of the combined modelling approach to assess its ability to simulate DO (section 4.1), followed by the sensitivity of DO to various nutrient input scenarios (section 4.2) and the decomposition of the dominant oxygen consumption and production processes along with the sensitivity of these processes to changes in input boundary conditions (section 4.3).

3.1 Evaluation of combined modelling approach

Figure 3 shows the simulated and observed DO concentrations at the four studied locations versus time. The Percent bias (PBIAS) and the Root Mean Square Error (RMSE) shown also in Figure 3 were used to give an indication of the match between observed and simulated DO concentrations. The PBIAS and RMSE equations are shown below:

$$PBIAS = \frac{\sum_{i=1}^{n}\left(Y_i^{Obs} - Y_i^{Sim}\right) * 100}{\sum_{i=1}^{n} Y_i^{Obs}}$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(Y_i^{Sim} - Y_i^{Obs}\right)^2}$$

Where Y_i^{Obs} and Y_i^{Sim} are the observed and simulated daily average DO concentrations respectively. The PBIAS assists in determining whether the model has a positive or negative bias. Positive values indicate underestimation, negative PBIAS indicate overestimation and zero PBIAS indicates a perfect match (Moriasi et al., 2007). Sint-Oedenrode and Hooidonkse Watermolen have negative PBIAS, showing that the model is slightly over predicting, while Bovenstrooms Effluentgoot and Genneper Watermolen have positive PBIAS indicating under prediction. The RMSE compares simulated and observed data and expresses the spread in $Y_i^{Sim} - Y_i^{Obs}$. The largest RMSE was obtained at Hooidonkse Watermolen while the smallest RMSE was obtained at Genneper Watermolen.

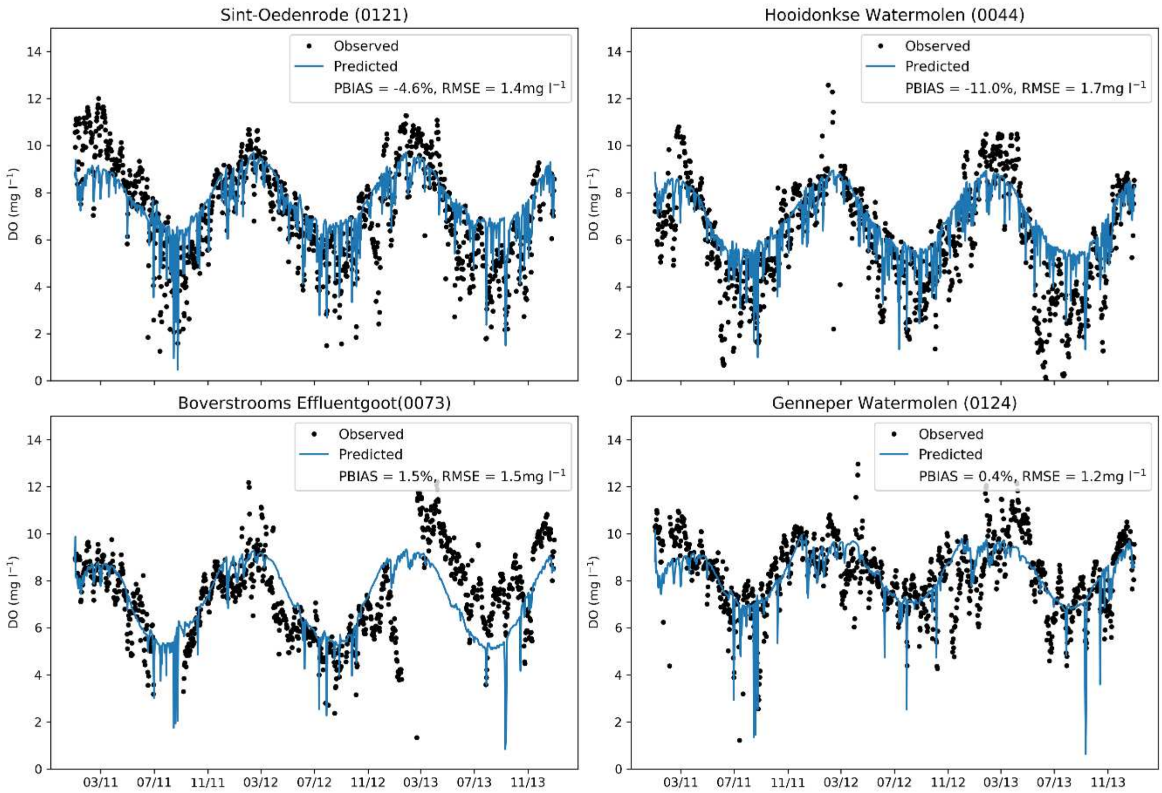

Figure 3. Simulated and observed dissolved oxygen concentrations versus time at various locations in the Dommel catchment (daily average)

Figure 4 shows the empirical cumulative distribution functions (ECFD) for the errors between the observed and predicted DO concentrations. Overall, there is a good match between simulated and observed concentrations. 83.9%, 87.9%, 71.1% and 84.2% of Sint-Oedenrode, Hooidonkse Watermolen, Bovenstrooms Effluentgoot and Genneper Watermolen predicted values were less than 1mg l^{-1} of the observed values, respectively. The largest differences between simulated and observed concentrations are observed in the recovery period following the DO falls from CSO events. This is shown by Figure 4 where EFCDs have longer tales towards the negative values. The observed DO concentrations at the Bovenstrooms Effluentgoot location after March 2013 systematically increased, potentially due to a monitoring error. These results suggest that the 'combined modelling approach' (referred as 'the model' for simplicity) can visually match the observed seasonal dynamics of dissolved oxygen. However, whilst the DO falls (due to oxygen depletion from CSO events) can be observed, their recovery is not fully captured by the model.

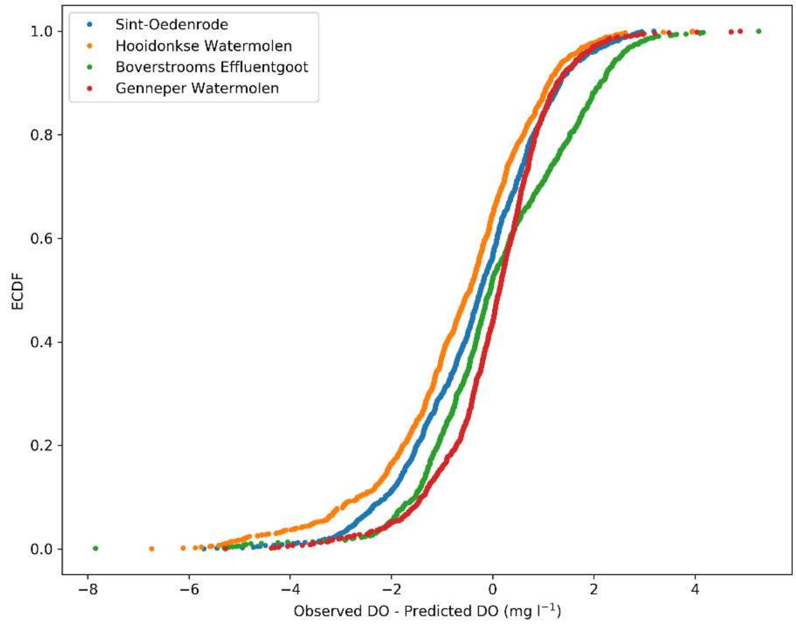

Figure 4. Empirical Cumulative Distribution Function (ECDF) of the difference between observed and predicted DO values.

3.2 Input Boundaries Sensitivity Analysis on Dissolved Oxygen Concentrations

The flow contributions from the boundary conditions (Rural runoff, CSOs, WWTP) are shown in Figure 5. It is important to note that Figure 5 does not show a hydrograph separation. It displays the precipitation as the average catchment precipitation, the total modelled flow at the outlet (Sint-Oedenrode), the sum of the surface and groundwater rural runoff inflows, the WWTP outflow into the Dommel upstream of the Bovenstrooms Effluentgoot sampling location, and the CSOs discharge inputs at various locations within the catchment. Figure 5 shows that the largest contribution of base flow arises from the rural inflows. These flows which are the main water inflow of the Dommel river are formed of fast surface runoff (activated during and after rainfall events) and slow groundwater baseflow. The next largest contributor of flow is the WWTP which has a constant base discharge of approximately 1.5 m^3s^{-1}. The WWTP has an overflow bypass storm settling tank which is activated during rainfall events, contributing additional flow to the river during and after rainfall events. The CSOs are significant contributors during precipitation events.

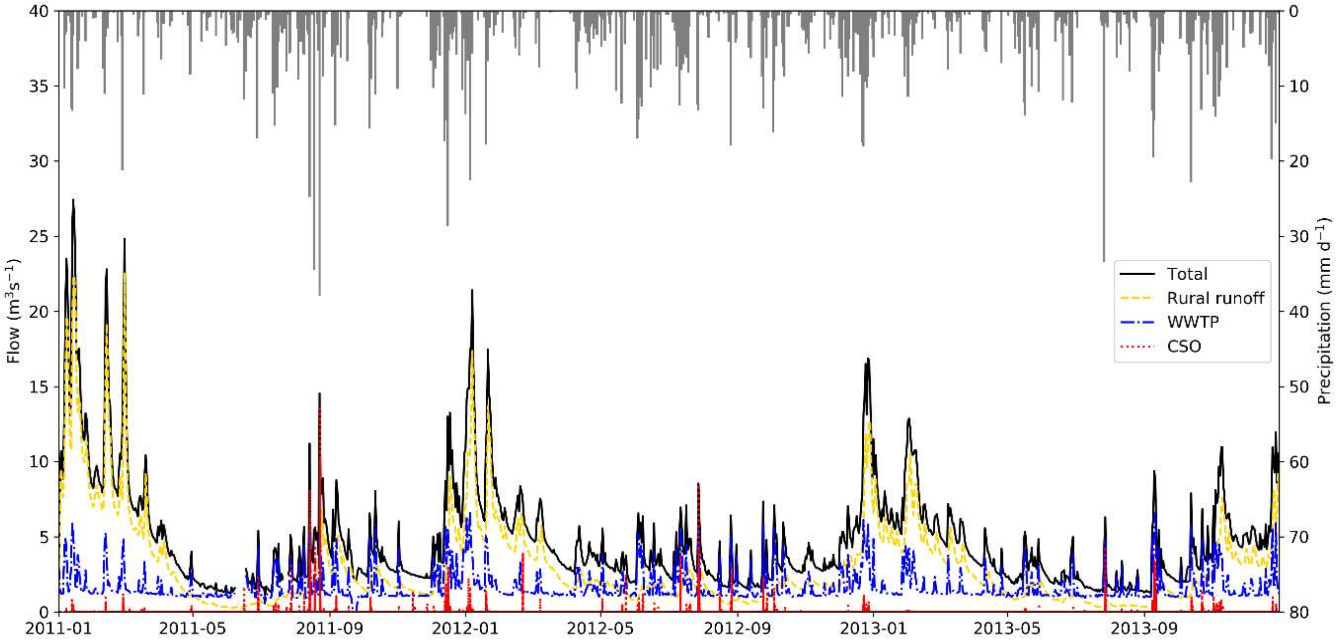

Figure 5. Daily flow average contributions in the River Dommel and Precipitation versus time

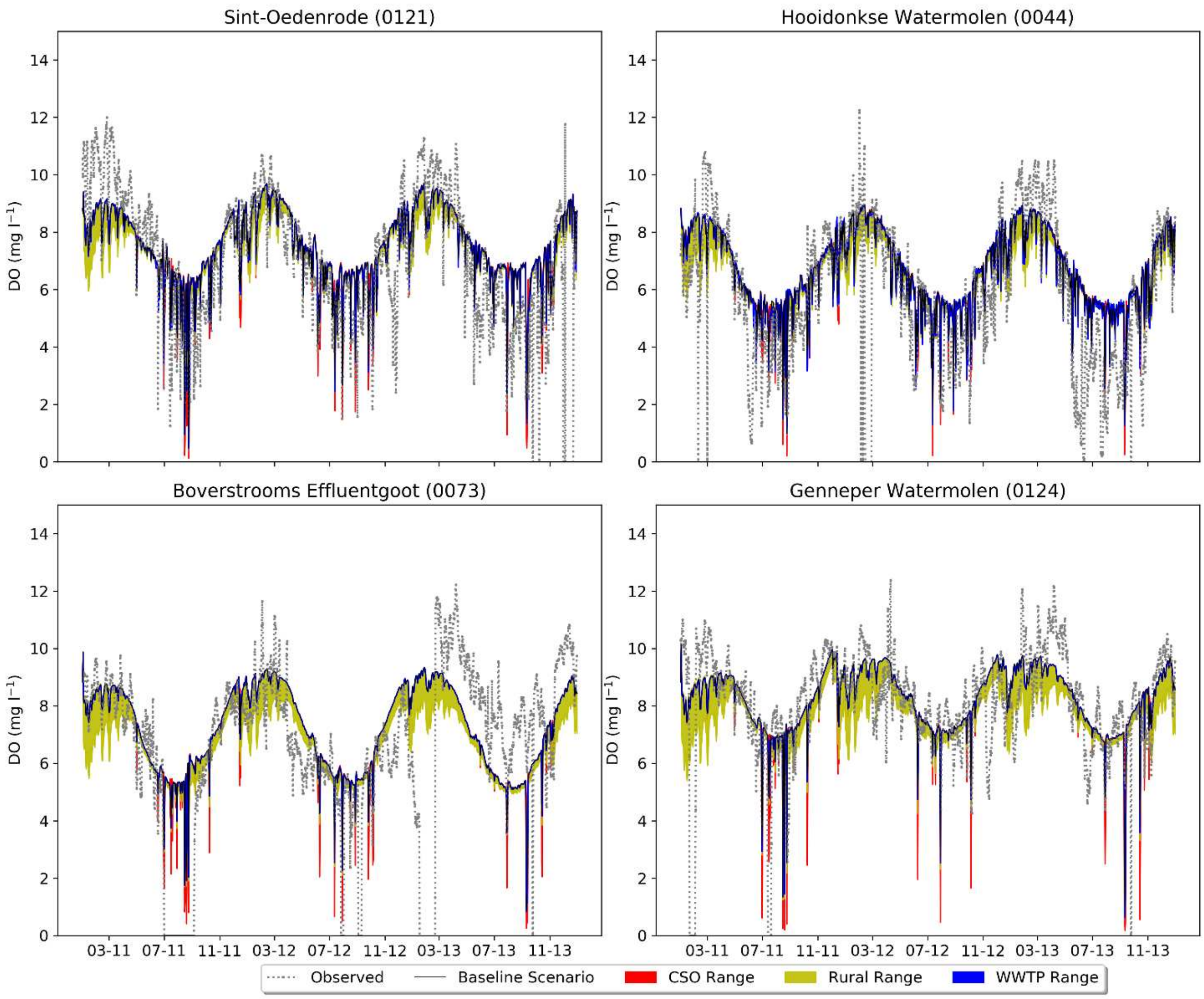

Figure 6. Sensitivity analysis results versus time. **The yellow, red and blue ranges correspond to the low and high ranges for the rural, CSOs and WWTP respectively.**

The sensitivity analysis results are shown in Figure 6. The baseline scenario represents the 'base' nutrient concentrations for the rural runoff, CSOs, and WWTP. The input concentrations for the rural and CSOs are shown in Table 3. The yellow, red, and blue areas display the ranges between the selected 'high' and 'low' scenarios of rural runoff, CSOs, and WWTP concentration levels, respectively. The seasonal influence of the rural runoff is observed in Figure 6 were the rural flows have a higher influence over the winter months. This effect is more noticeable in the upstream locations (Boverstrooms and Genneper Watermolen) where the catchment is less urbanized. Most of the connected urban area is located in the downstream sections at the Eindhoven city. The influence of the CSOs is visible during precipitation events. The short term CSO effects are expected since these occur due to excess of drainage capacity during rainfall events. Moreover, the oxygen depletion occurrences due to the CSOs have severe acute effects on the river ecology. The high and low scenarios of WWTP input concentrations have the lowest impact over the DO concentrations, and do not impact the Boverstrooms and Genneper Watermolen locations since these do not receive flow from the WWTP.

3.3 Dominant Processes in Oxygen Production and Consumption

The sources and sinks of dissolved oxygen (DO) in the Dommel River at Sint-Oedenrode are shown in Figure 7 and Figure 8. These illustrate the daily production and consumption of DO for the simulated period from 2011 to 2013. The sum of these processes results in the daily concentration contribution that was produced or consumed. In addition, Figure 7 and Figure 8 show the ranges of concentrations obtained when the low and high scenarios of boundary conditions are analysed. The yellow, red and blue correspond to the low-high ranges for the rural, CSOs and WWTP respectively.

Figure 7 reveals that aeration is the main source of DO, followed by the production of oxygen by phytoplankton, and macrophytes production. The contribution of DO from aeration is higher than the contribution of DO from macrophytes production and production by NO_3 uptake by macrophytes by several orders of magnitude. Aeration remains fairly constant throughout the simulation except for when CSOs occur when aeration may increase up to 7 mg $l^{-1}d^{-1}$. This is expected due to turbulent flows entering the river from the CSOs during and after rainfall events.

Figure 8 shows that the dominant consumption processes consist of mineralization and nitrification of detritus (in water and the sediment) and respiration of macrophytes and phytoplankton.. Higher mineralization processes are expected in the Dommel due to the high organic loads coming from both rural runoff and CSOs.

The macrophytes processes of production, and NO_3 uptake display a seasonal pattern in which vegetation suddenly increases during the spring/summer. However, the effect of mowing is highly noticeable by the sudden drop in production and NO_3 uptake on June 1st of each studied year (when mowing occurs). After mowing, the remaining vegetation starts to increase again until winter arrives, and the vegetation reduces once again. Moreover, the peaks of macrophytes production and NO_3 uptake, and dips in macrophytes respiration become progressively smaller over the three years that were simulated, indicating that with the current simulated mowing regime the vegetation appears to be incapable of fully recovering after mowing.

The sensitivity of the system to changes in input boundary conditions (low and high levels of nutrient scenarios) is visible in Figure 7 and Figure 8. The rural runoff (yellow range) has a constant impact over aeration throughout the studied time, while the CSOs (red range) have specific impacts on aeration which are evident by the aeration spikes which occur during and after precipitation events. The macrophytes processes are more sensitive to CSOs impacts than the other boundary conditions. This is expected to be due to the organic loads within CSOs. Although CSOs occur at daily or sub-daily timescales, the organic loads remain in the system and decompose throughout time, reducing the oxygen available for vegetation. Mineralization and nitrification processes are sensitive to all boundaries. Particularly, rural nutrient input is constantly reflected in nitrification. In addition, sudden drops in nitrification are also noticeable due to WWTP input.

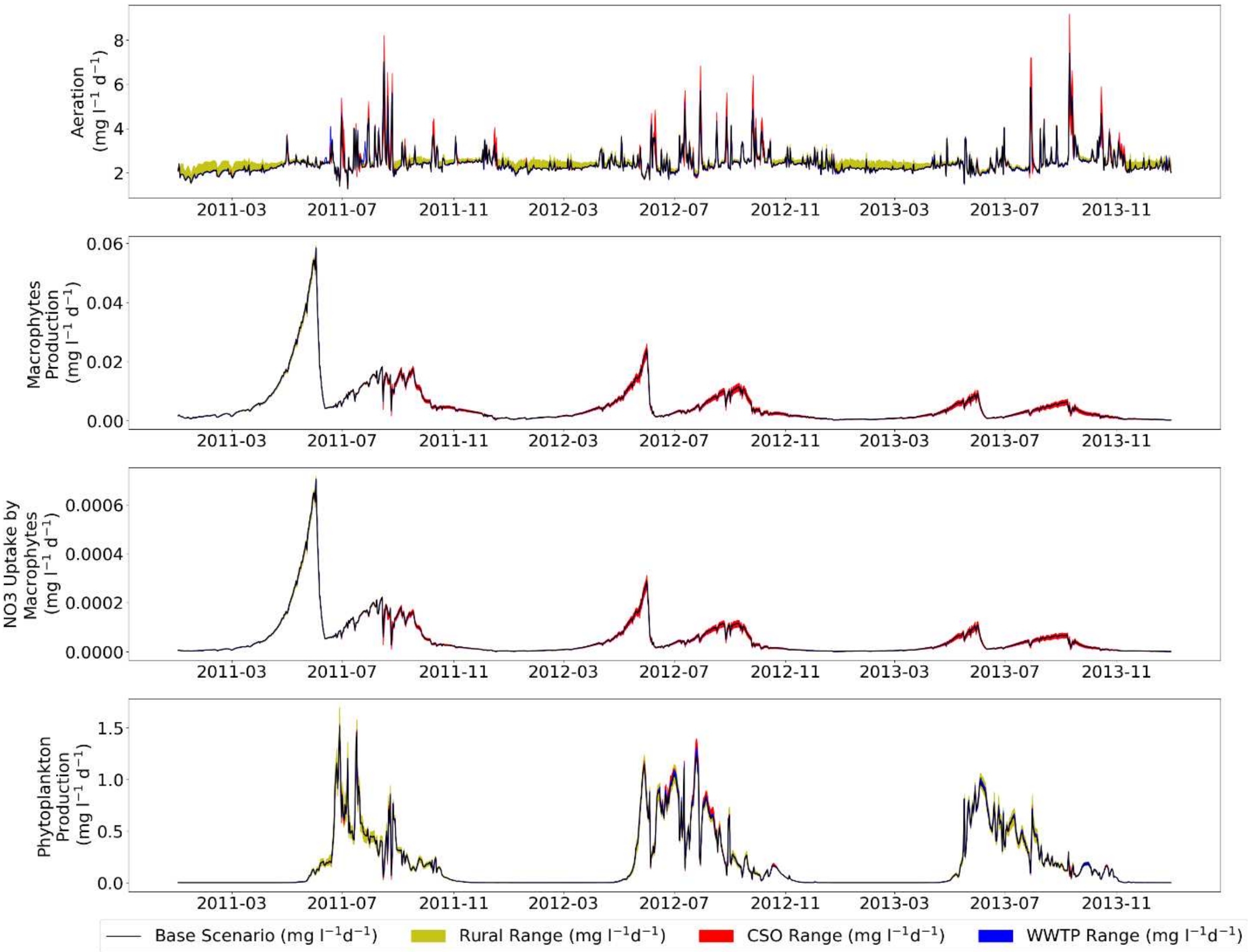

Figure 7. Dissolved Oxygen production processes versus time and sensitivity of boundary input scenarios. The yellow, red and blue ranges correspond to the low and high ranges for the rural, CSOs and WWTP respectively.

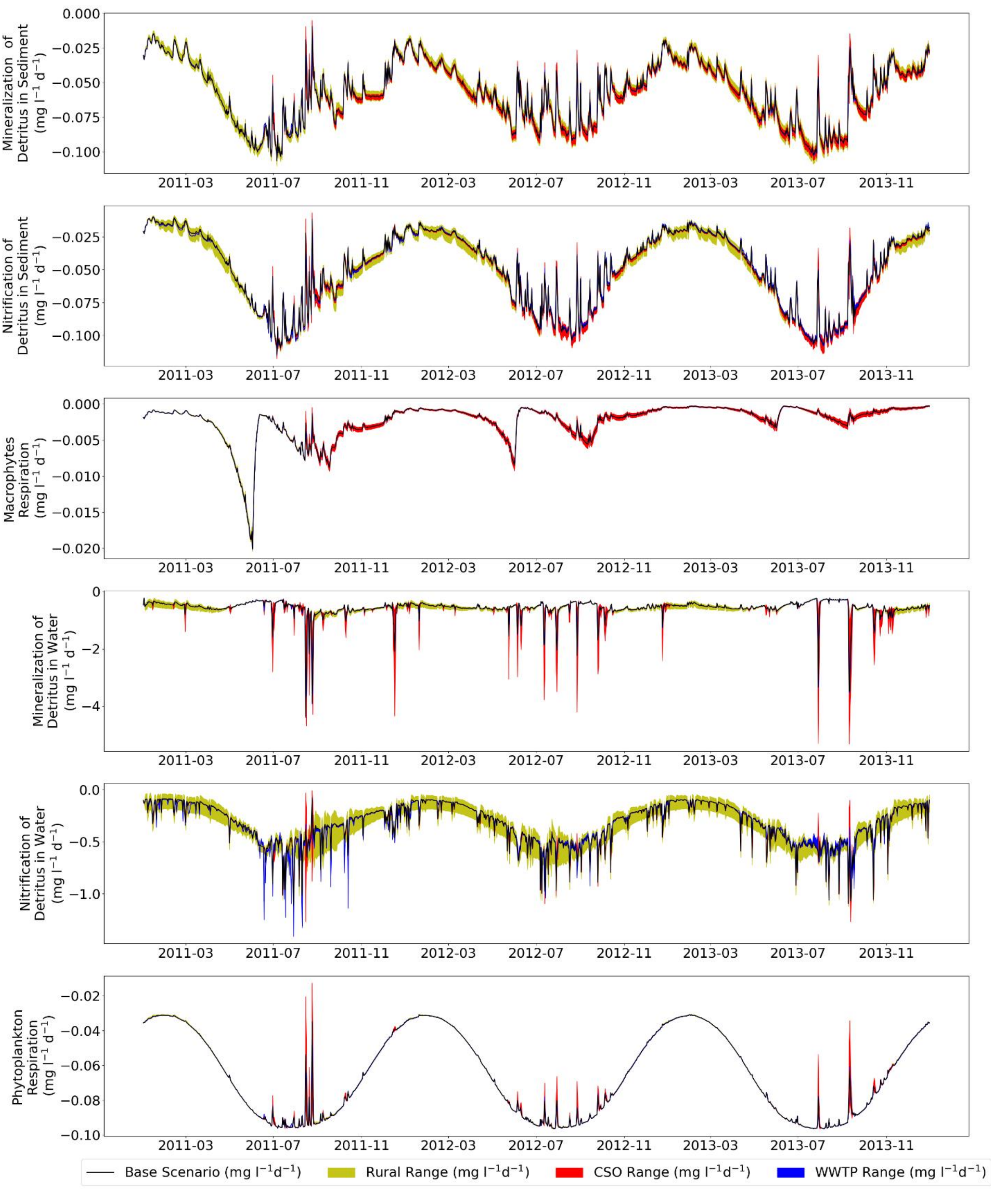

Figure 8. Dissolved Oxygen consumption processes versus time and sensitivity of boundary input scenarios. The yellow, red and blue ranges correspond to the low and high ranges for the rural, CSOs and WWTP respectively.

4 Discussion

This study combined a rainfall-runoff model, hydrodynamic model and closed-nutrient cycle model to simulate DO concentrations for the Dommel River, and their sensitivity to low and high scenarios of nutrient inputs. In addition, the oxygen decomposition into the production and consumption processes was carried out along with the sensitivity of these processes to changes in nutrient levels.

The first aim of the paper, to evaluate the combined modelling approach (from now on referred to as 'the model'), demonstrated that the methodology can be used to simulate the seasonal dynamics of DO. The DO concentrations were the highest during the winter months and lowest during the summer months potentially due to higher solubility during high flow. The model matches this winter/summer dynamic with low values of Root Mean Square Errors ranging from 1.2 to 1.7 mg l^{-1}, and PBIAS values ranging from -11.0% to 1.5% despite some measurement errors in the observed data (Figure 3). Accurately estimating the seasonal behaviour is necessary when evaluating the long term effects of eutrophication.

The model, however, is not as suitable for simulating the short term dynamics of DO since it cannot fully capture the DO depletion and recovery events (Figure 3). This is partly due to the inability of the ecological model PCDitch to have a higher time resolution than the daily time resolution used in this study. The lack of representation of these DO falls and their recovery might also be due to the absence of slow degradation of organic matter.

In addition, the current model implementation does not explicitly represent mixing processes such as dispersion, transient storage and hyporheic exchange. This is based on the assumption that mixing processes within the river occur within the sub-daily time scales, and therefore that the performance of the model will be relatively insensitive to the representation of mixing processes when assessed against daily observations. However, it is recognised that a more detailed representation of these processes are likely to be significant when considering the temporal dynamics of aquatic ecosystems more detailed (sub-daily) temporal resolutions. This may require a more detailed calibration of dispersion coefficients (Camacho Suarez, 2019) and/or inclusion of transient storage and hyporheic exchange (Runkel, 1998; Ryan and Boufadel, 2007). Furthermore, the modelling approach implemented within this study can be coupled with a higher temporal resolution DO model to simulate shorter periods if this is the main interest or purpose of the user thus providing boundary conditions for higher temporal resolution models. For instance, Moreno-Rodenas et al. (2017) carried out an integrated catchment modelling study in the Dommel River. With a focus on determining the impact of the spatiotemporal effects of rainfall variability, they evaluated the dissolved oxygen concentrations in the Dommel River. Their Integrated Catchment Model (ICM) included a rainfall-runoff model which was complemented with the urban components of CSOs and the WWTP and a water quality module. The processes of fractionation of Biological Oxygen Demand, respiration from macrophytes and nitrification-denitrification were included in the water quality module in a three-phase layout module to account for the atmosphere-water-sediment interactions. In contrast to the study presented in this paper, Moreno-Rodenas et al. (2017) focused on shorter time scales studying particular rainfall events. These allowed to better understand the dynamics of the CSOs, and the WWTP in response to the precipitation events. However, such models require more computational resources for a long term eutrophication study evaluation, have a reduced representation of the modelling system (by integrating less ecological processes and components), and do not provide insights regarding the ecological processes involving the aquatic biota.

The sensitivity of the DO concentrations, and the DO consumption and production processes in response to changes in nutrient levels at the boundary conditions was analysed (Figure 6, Figure 7 and Figure 8). The varing influence of the rural runoff over the year is noted in Figure 6, with rural impacts being dominant during winter months. This is in contrast to the influence of CSOs, which are significant during shorter term rainfall events. Both, short and long-term effects have consequences over the river habitat. The short-term

DO depletion caused by the CSOs may have acute effects (lethal for fish/macro fauna) while the while seasonal lowering of oxygen concentration affects the habitat, meaning that oxygen sensitive species will not be abundant in the river basin. The discharge of the WWTP flow in the river appears to have a smaller impact over the DO concentrations at the Hooidonkse Watermolen and Sint-Oedenrode locations, even though the WWTP is a major contributor of flow to the river system (figure 5).

Figure 7 and Figure 8 illustrate how the sources and sinks of DO behave seasonally and in response to the changes in boundary conditions. The decomposition of dissolved oxygen processes shows that aeration is the main source of DO into the river system with values ranging from 1.5 to 7 mg l^{-1}. Aeration is also sensitive to changes in the boundary conditions of rural runoff and CSOs. When organic loads from both rural runoff and CSO's, enter the water system, water depth is affected, causing increased flows and turbulence in the system which will lead to spikes in aeration.

Figure 8 shows the influence of the rural runoff and the CSOs over the mineralization and nitrification of detritus in the water and also in the sediment. This is due to the inflow of suspended solids contributing to both, organic and inorganic matter into the system. Most of the organic matter in the system will settle into the sediment and decompose contributing to the mineralization and nitrification processes. The mineralization of detritus in the water column is sensitive to the CSO events resulting in spikes of DO depletion. The wastewater treatment plant mainly affects the nitrification processes in the water column by the WWTP discharges of ammonium in the water system. The remaining organic matter mainly consists of humidic acids, which are slowly to not degradable and do not cause a significant and direct oxygen demand in the water column. These interactions between nutrient inputs and oxygen processes show that the system, already loaded by high organic matter content, is likely to tip on to a low oxygen state as observed in a study by Veraart et al. (2011).

Vegetation is significantly affected by mowing. The sharp decrease in macrophytes production in Figure 7 is due to mowing every June 1st. Consequently, the vegetation recovers over the summer but dies during the winter months. It is noted that this particular mowing scenario is removing more vegetation faster than the system can replenish itself. This effect is also visible for the macrophytes respiration and NO_3 uptake. This supports the view that vegetation management strategies can have a substantial effect on water quality and ecological function in river systems. The modelling approach also showed that vegetation is sensitive to CSO events (Figure 7 and Figure 8). A constant influence of the CSOs is noted over the macrophytes DO production.

Overall, the advantages of using PCDitch over other water quality models is noted by this study where the decomposition of dissolved oxygen process and the sensitivity analysis of the boundary inputs revealed critical interactions such as the importance of the CSOs over vegetation, the influence of rural runoff and the WWTP discharge on nitrification, and the sensitivity of the system to the removal of vegetation. This modelling approach is capable of providing an overview of the river processes due to its ability to include the various ecological processes such as the competition of vegetation for nutrient, lights, and temperature. Other models, for instance the Charisma model (van Nes et al., 2003), are also able to model the competition of plants. However, only two types of submerged vegetation are included in the Charisma model (McCann, 2016) while PCDitch incorporates six types of aquatic vegetation. Capturing such vegetation density and its relationship to flow dynamics has been recognized to assist in assessing the ecological quality of the water system (Kuipers et al., 2016), and this is attainable with this modelling approach by coupling the hydrodynamic and ecological models. Furthermore, PCDitch describes the relation between external nutrient loadings, nutrient concentrations and the dynamics of the different types of vegetation (submerged plants, algae, duckweed and helophytes).

5 Conclusion

This work evaluates a combined modelling approach to describe hydrologic, hydrodynamic and ecological processes within a catchment in order to provide a holistic view of a river system and its sensitivity to both urban and rural inputs. Such integrated approach is crucial for the full assessment of the catchment and implementation of management measures in response to human pressures. In this study, the modelling approach is evaluated based on a rural and urban catchment (the Dommel River catchment). Precipitation evaporation, and runoff inputs were modelled using a rainfall-runoff modelled designed for low-land areas, followed by the hydrodynamic simulation which included CSOs, the Eindhoven treatment plant and other urban components. The novelty of this study lies in the successful implementation of the extensive closed-nutrients cycle model to the slow flowing river highly impacted by urbanization and rural inputs. PCDitch, which was initially developed for ditches, was used to model DO concentrations for the first time. In addition, this paper studies the decomposition of oxygen processes into production and consumption processes and their sensitivity to low and high levels of nutrient inputs from the different boundaries given mowing and dredging in the river system.

This study found that the seasonal pattern of dissolved oxygen can be well simulated with the combined modelling approach, although some shortcomings are identified when modelling DO recovery following CSO events. Secondly, the sensitivity of the dissolved oxygen processes to changes in nutrient high and low levels from the boundary conditions showed that DO levels are influenced by rural runoff mainly during the winter months. This influence is more notorious in the upstream locations. In addition, it was observed that the CSOs have short-term impacts over DO during and after precipitation events. Thirdly, the separation of oxygen processes into the production and consumption processes and sensitivity analysis revealed: i) a continuous influence of the CSOs input concentrations on the vegetation processes of production, respiration and NO_3 uptake, ii) an influence of rural runoff over nitrification and mineralization processes, iii) a sharp impact of mowing on vegetation processes, and iv) an intermittent effect of the WWTP on mineralization during and after precipitation events.

The model structure of PCDitch using closed nutrient cycles allows for a better understanding of the nutrient dynamics within the ecological habitat allowing the study of important ecological processes affecting the production and degradation of oxygen while implementing vegetation and dredging management practices. This allows for a deeper consideration of such important processes into river management strategies than is currently possible.

These findings are an illustration of the knowledge that can be gained from a modelling approach which incorporated both hydrological, hydrodynamic and detailed ecological processes. With such understanding, specific urban or rural management measures may be more fully considered to improve the overall health of the river system.

Acknowledgments

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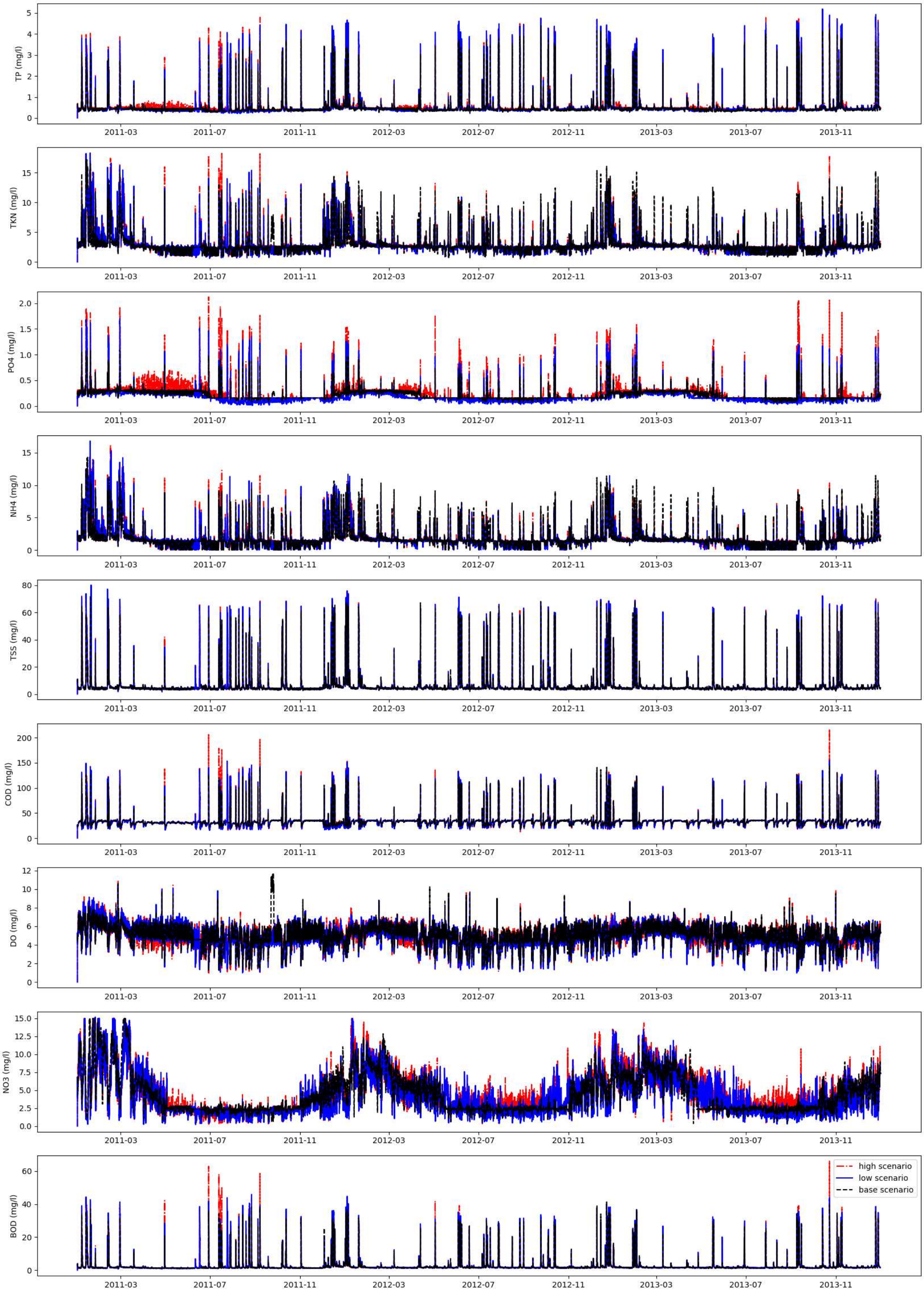
Appendix A: Simulated WWTP nutrient input scenarios



Appendix B: WALRUS model results and calibration

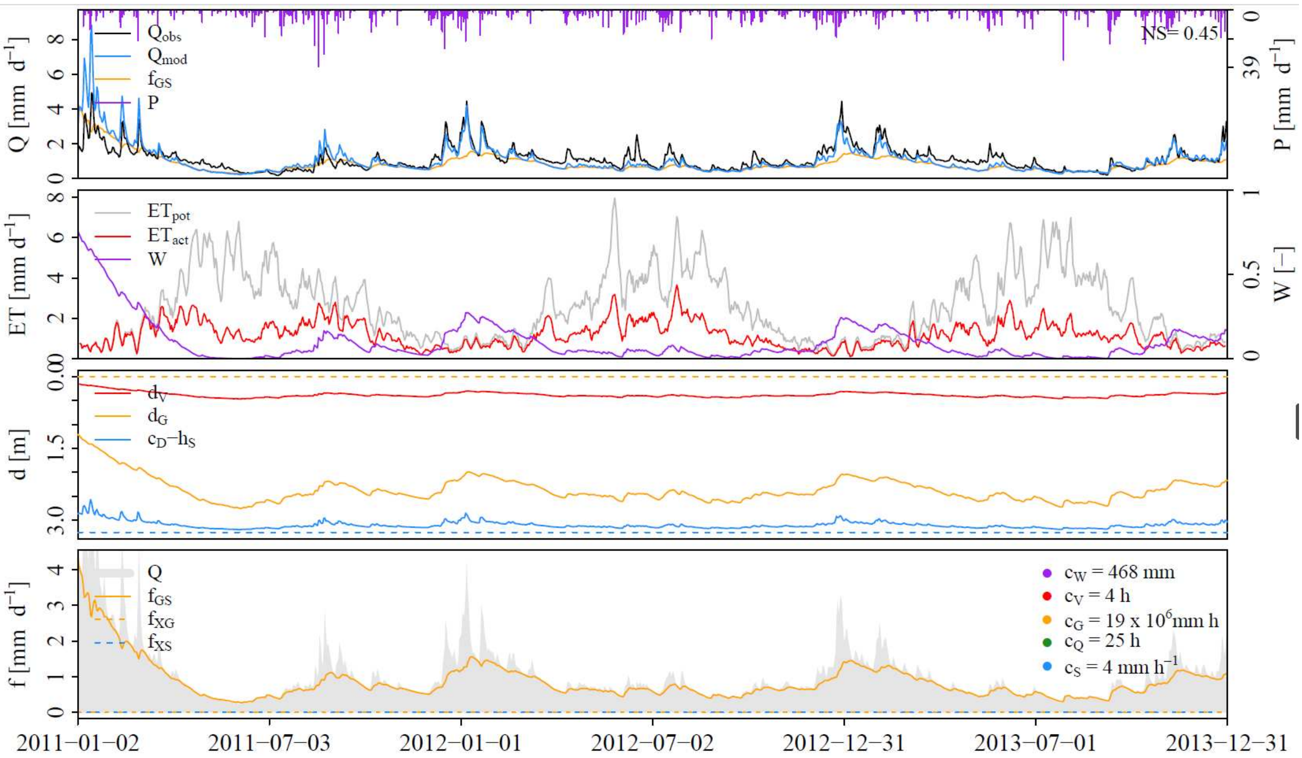


Figure B1. Walrus model results and calibration for Keersop catchment

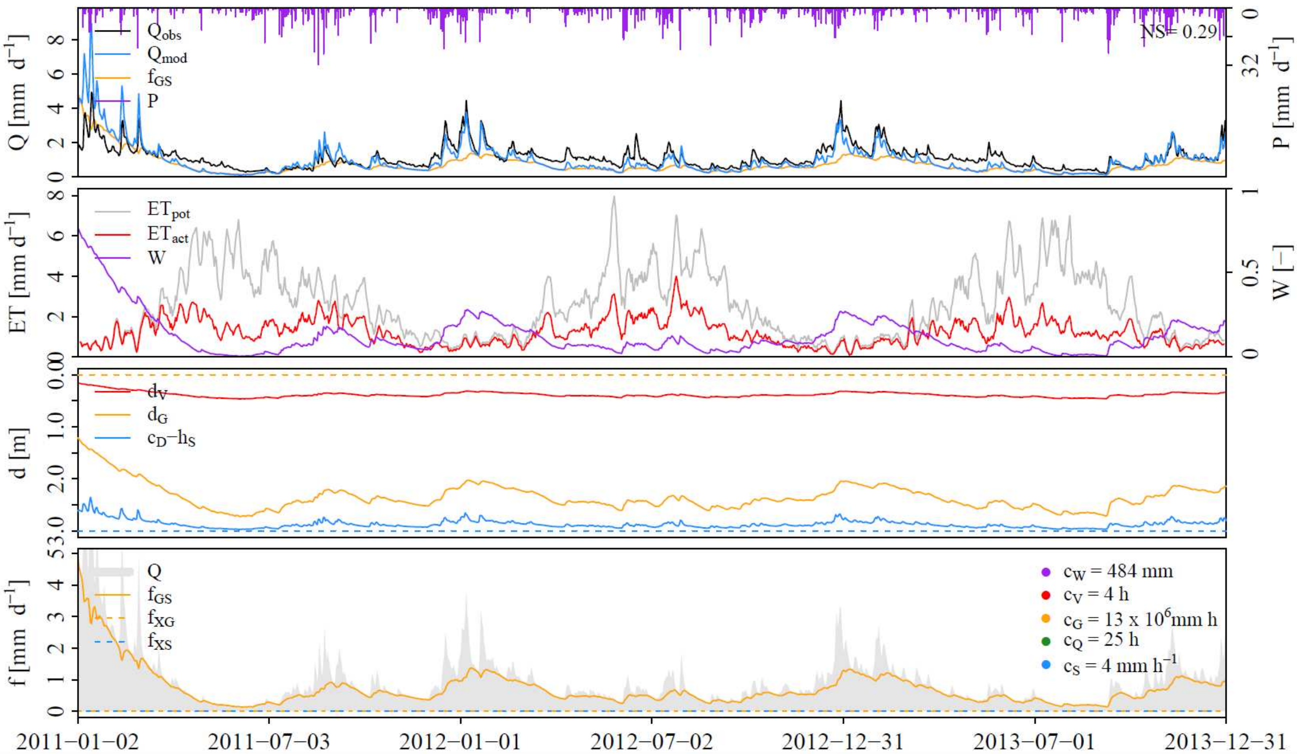


Figure B2. Walrus model results and calibration for Tongelreep catchment

Appendix C: Observed and predicted flow using Sobek hydrodynamic model