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Research papers

Coupled hydrologic, hydraulic, and surface water quality models for pollution management in urban–rural areas

Matteo Masi [a,*], Daniele Masseroni [b], Fabio Castelli [a]

[a] Department of Civil and Environmental Engineering, University of Florence, Via di S. Marta 3, 50139, Firenze, Italy
[b] Department of Agricultural and Environmental Sciences, University of Milan, Via Celoria 2, 20133 Milan, Italy

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ABSTRACT

Urban expansion and increasing frequency of extreme events threaten both urban drainage and receiving waterbody water quality. Combined sewer systems are particularly vulnerable, as they mix wastewater and stormwater, making them susceptible to reduced drainage efficiency and potential release of pollutants. Nature-based solutions, such as constructed wetlands, offer an effective means of pollution mitigation by providing sustainable and cost-efficient methods for enhancing water quality and reducing pollution in urban environments. This study presents a numerical modelling framework to simulate the impact of pollution and to design effective remediation strategies in mixed urban–rural networks subjected to storm events. The model consists of three main modules integrating hydrological, hydrodynamic, and reactive transport components to simulate the water and pollutants dynamics. The first module simulates runoff based on a distributed hydrological model and propagation within the canal network. A reactive transport module simulates advective–dispersive transport and biochemical reactions of pollutants. A third module evaluates the effectiveness of horizontal flow constructed wetlands for pollution mitigation. The model is applied to a suburban area near Milan, Italy, where sewer overflows enter a network of irrigation canals. The results demonstrate that the model was effective in identifying a suitable location for implementing a constructed wetland and in determining its proper size to achieve improved water quality. According to the simulations, the designed treatment system can achieve a contamination reduction of up to 23% for ammonium, 84% for nitrates, and 85% for carbonaceous BOD.

1. Introduction

The rapid and heterogeneous expansion of many urban areas, associated with increasing frequency of extreme events, may significantly affect the operational capacity of urban drainage systems. The consequences of such trends affect the rainfall-runoff processes and pollutant fate and transport in surface waters. These effects are particularly relevant for combined sewerage systems (CSSs) where wastewater and rainwater mix. During severe rainfall events, the effluent flowrate can exceed the interception capacity of the sewerage system, resulting into the discharge of untreated water into the receiving water bodies (Botturi et al., 2021). Consequently, combined sewer overflows (CSOs) have been identified as significant contributors to flooding (Jean et al., 2018; Masseroni et al., 2018) and water pollution (Li et al., 2022; Madoux-Humery et al., 2016; Spill et al., 2023) of receiving water bodies (RWBs).

The assessment of the impacts of CSOs on RWBs should take into account processes occurring at different spatial and temporal scales, especially in agro–urban contexts, i.e., where urban drainage systems and rural hydraulic networks overlap. In this complex scenario, the issue of pollutants spreading within the waterway systems emerges as crucial for the examination and adoption of approaches aimed at regulating, managing, and treating CSO water. Implementing nature-based solutions (NBS), such as constructed wetlands (CWs) for CSO water treatment offers significant benefits, including improved water quality through the removal of conventional pollutants, pathogens, and emergent contaminants, while also providing ecosystem services and long-term sustainability for urban water management (Rizzo et al., 2020). The effective evaluation of the influence of these overflows on the water bodies they discharge into and the correct design of mitigation solutions, rely on the knowledge of pollutant concentrations and their propagation along the network. It is beneficial to use mathematical models that allow to reconstruct and predict the interconnected relationships between water quantity and water quality (Bai et al., 2022). In such systems, combining modelling tools that connect processes at watershed *meso-*

* Corresponding author.
E-mail address: matteo.masi@unifi.it (M. Masi).

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scale (Gillefalk et al., 2022) and hydrodynamic and reactive-transport simulations at the river scale is a challenging task in term of complexity (Keller et al., 2023) and multiple processes coupling (Debele et al., 2008; Mannina & Viviani, 2010).

Several authors have undertaken the coupling of different models to concurrently assess hydrologic, hydraulic, and water quality processes in various scenarios, though typically outside the scope of urban–rural water networks. Mesquita and Lima Neto (2022) evaluated the hydrological processes, hydrodynamics, and water quality dynamics in an urban lake in Brazil to assess the impact of water pollution on lake evaporation. Xue et al. (2015) developed an urban river water quality model which includes the river physical-biochemical processes and the incorporated urban catchment rainfall-runoff process. Brito et al. (2018) integrated a reservoir water quality model (CE-QUAL-W2) and a hydrologic model (SWAT) to simulate the reservoir state and to test management measures for reducing trophic levels and algal bloom peaks. Debele et al. (2008) integrated SWAT and CE-QUAL-W2 to simulate water quantity and quality processes from upland watershed to downstream water bodies.

Recently, several studies used machine learning approaches to predict water quality both in urban and rural environments. Zhao et al. (2020) employed principal component and fuzzy approaches to couple urban river water quality with water quantity models. Schäfer et al. (2022) demonstrated the use of machine learning techniques, specifically boosted trees and generalized additive model (GAM), to analyse water quality dynamics in the urbanized River Chess, highlighting the influence of wastewater treatment outflow on electrical conductivity and temperature variations. Xue et al. (2024) presented a machine learning framework using random forest to predict nitrogen and phosphorus concentrations in rivers, specifically in an urban–rural transitional area in Wenzhou, China, addressing water quality issues related to rapid urbanization and non-point source pollution. However, machine learning models training and validation rely on large datasets collected from public services, monitoring stations, or available measurements, which are often scarce or inaccessible (Cojbasic et al., 2023).

While previous studies have successfully coupled hydrological, hydraulic, and water quality models (Bui & Pham, 2023) or applied machine learning to predict water quality under specific scenarios (Zhu et al., 2022), these efforts often focus on isolated processes or specific contexts, such as urban environments (Zhang et al., 2022) or large-scale catchments (Sadayappan et al., 2024). They do not fully address the interconnected dynamics of water systems at multiple scales, including the role of nature-based solutions in managing water resources across urban–rural networks.

Run-off and transport mechanisms during an event that leads to CSO discharge into RWBs require to be modelled as unsteady processes (Ferreira et al., 2019). At the watershed scale the rainfall-runoff simulation is intrinsically a nonstationary problem which can be addressed by several available hydrologic tools. However, at the river scale, many of the available surface water quality modelling tools, such as QUAL2E, QUAL2K, TOMCAT, SIMCAT, lack the capability for variable flow simulations (Ranjith et al., 2019). Conversely, other tools designed for variable flow simulations, such as WASP8, QUASAR, are specifically developed for river modelling but face limitations when applied to networks with complex topologies, or coupled with watershed-scale processes. The One-Dimensional Transport with Inflow and Storage (OTIS) model, developed by the USGS, is another tool for simulating water quality and quantity in rivers. Although OTIS is a powerful and flexible modelling tool that can integrate hydrologic processes and chemical reactions, it is not designed for direct application to mixed networks of pipes and channels. Models like SWAT and SWMM offer the advantage of coupling watershed and river hydrodynamics. While SWAT focuses on watershed scale processes, its limitation in dealing with fast runoff events due to its daily time step may make it unsuitable for certain applications. In particular, the SWAT model may not be the most appropriate choice for modelling complex urban networks of pipes and channels. SWMM emerges as a promising option for such networks, although it also has notable limitations, which are discussed below.

Having both mixed urban and rural systems drainage in the modelled area implies that in some regions of the network transport regime may be advection-dominated, e.g., in pipes or regular channels, while in other points of the network where small flow velocities occur, dispersion may become a relevant transport mechanism (Ji, 2017). Consequently, in agro-urban environments, the role of dispersion in species transport cannot be disregarded. Despite SWMM's popularity as a water quantity and quality model for networks of pipes and channels, its transport model relies on a simplified transport model based on Continuous Stirred Tank Reactors (CSTR) in series, in which dispersion coefficients are not explicitly considered. Indeed, the structure of the model through a combination of CSTR implicitly introduces a numerical dispersion (Socolofsky & Jirka, 2005), which may not reflect the actual dispersion phenomena occurring in the real system. Therefore, enhancing the transport model's accuracy necessitates the incorporation of dispersion coefficients, which can be measured or predicted by means of appropriate empirical formulas (Peruzzi et al., 2021). In addition to advection, diffusion, and dispersion, the non-conservative species in water system undergo transformations due to various processes, such as chemical reactions, physical processes like particulate settling, and biological processes such as algae growth and death, resulting in either loss or gain of mass (Ferreira et al., 2020). These reactive processes are thoroughly addressed in specialised water quality software such as QUAL2K and WASP, while they are not as prominent in models that focus primarily on quantity like SWMM.

Among the various strategies to mitigate pollution transported by rivers and channels, the constructed wetlands (CW) are engineered systems, which use physical, biochemical and physiological processes of natural wetlands to control water pollution (Kadlec & Wallace, 2008). They have been successfully employed for removing a wide range of pollutants from wastewater, runoff water, and agricultural drainage water (Lavrnić et al., 2020; Sabri et al., 2021; Vymazal & Březinová, 2015). Among the different typologies of CWs, the horizontal flow constructed wetland (HFCW) is a common type to treat organic loads (Hassan et al., 2021). Processes and removal mechanisms in HFCWs, and in CWs in general, include a large number of chemical, biological and physical mechanisms, that can occur simultaneously and interconnectedly (Langergraber & Šimůnek, 2005). Modelling of CWs is a complex task due to the necessity of describing numerous processes, which can be grouped into the following main components: the water flow, the transport model, the biochemical model, the plant model and clogging processes (Langergraber & Šimůnek, 2018). Being very complex systems, the design of CWs is generally performed using simplified models and empirically derived parameters (Mena et al., 2008). More advanced models, such as CWM1 (Langergraber et al., 2009), have been developed to provide a detailed representation of the reactive processes occurring in CWs. While CWM1 has been successfully integrated with the hydrodynamic simulation code HYDRUS (Rizzo et al., 2014), there are currently no examples of its integration within a comprehensive framework that combines hydrologic, hydrodynamic, and reactive transport modeling.

The limitations of existing reviewed models suggest the need for a new modelling framework that can comprehensively assess water quantity, quality, and mitigation strategies in complex urban–rural drainage systems.

In this study, we present a coupled hydrological, hydrodynamic and reactive transport model for simulation of the effects of surface water pollution in mixed urban–rural networks during rainfall events and their mitigation through nature-based treatment systems. We built the modelling framework upon the existing model MOBIDIC–U (Ercolani et al., 2018) originally designed for simulating runoff and water flow in urban canal networks, by significantly enhancing its functionality. The key improvements include: (i) adapting the original code to extend its applicability to rural areas, (ii) implementing a reactive-transport module to simulate the advective and dispersive transport and biochemical reactions of pollutants in the network, and (iii) developing a dedicated software module to simulate the pollution mitigation capacity of horizontal flow constructed wetlands (HFCW).

We demonstrate the application of the model to a case study located in a suburban area of Milan (Italy) to evaluate the effects of sewerage overflows and runoff on the water quality status of the RWBs. Additionally, the model is used to evaluate the application of HFCWs to mitigate the pollution and to achieve water quality standards suitable for agricultural and other reuses.

2. Materials and methods

2.1. Modelling framework

The modelling framework is based on MOBIDIC ("MOdello di Bilancio Idrologico DIstribuito e Continuo" – distributed and continuous hydrological balance model). MOBIDIC is a distributed and raster-based hydrological balance model that represents the hydrological cycle by simulating energy and water balances on a cell basis (Castelli et al., 2009; Yang et al., 2014). MOBIDIC was originally developed to simulate processes at the catchment's scale for floods forecasting and water resources management purposes (Campo et al., 2006). In later studies, the software was adapted for the simulation of runoff formation and propagation in the urban environment (MOBIDIC–U), by adding the following features (Ercolani et al., 2018): (i) the description of drainage network though a coupled system of polylines (conduits) and points (nodes) vector layers, (ii) the flow routing through the drainage network and mass conservation in the nodes, (iii) a modified approach for surface runoff routing considering that flow path in the urban environment is rarely determined by terrain slope, and (iv) the simulation of low impact development solutions (LIDs).

In this work, the MOBIDIC–U model has been enhanced and evolved into MOBIDIC–UR to broaden the scope of simulations, now encompassing both urban and rural channel networks. The enhanced MOBIDIC–UR software introduces several key capabilities that distinguish it from the original MOBIDIC–U package. These include: (i) an algorithm for automatically extracting cross-sectional profiles (elevations and geometries) directly from digital elevation models (DEMs), (ii) the ability to model channels with trapezoidal cross-sections, and (iii) support for incorporating external flow rates at network nodes, enabling the simulation of features such as combined sewer overflows (CSOs).

Additionally, two new modules were developed: MOBIDIC–UR–ADR (Advection–Dispersion–Reaction module) and MOBIDIC–UR–CW (Constructed Wetland module), which allow for the simulation of reactive-transport, and pollution mitigation through constructed wetland treatment systems, respectively. The modeling framework is entirely written in the MATLAB programming language. The software architecture and the required model inputs are shown in Fig. 1.

In the main module MOBIDIC–UR, the hydrological processes, both parameters and results, are represented with a fully distributed approach for which a raster-based discretization of the area of study is required. The required computational inputs are the digital elevation data (DEM) and the geo-processed hydrological parameters (flow direction and flow accumulation). In the model, soil is vertically represented as a single layer, with a conceptual subdivision into two non-linear interconnected reservoirs corresponding to larger pores draining water under gravity (gravitational reservoir) and smaller pores holding water through capillary forces (capillary reservoir). The storage capacity of the two reservoirs are parametrized as the maximum water content above field capacity ($W_{g,max}$), and the difference between field capacity and residual water content ($W_{c,max}$), respectively. Additionally, water interception (e.g., by vegetation) is described by another reservoir characterized by a finite volumetric capability ($W_{p,max}$). A comprehensive description of the model is given by Ercolani et al. (2018).

The hydraulic module of MOBIDIC–UR conceptualizes the physical elements of the pipes and channel network into a set of nodes and links. The nodes are points that represent junctions, inlets or outfalls, while links represent pipes and channels which connect nodes to another. The flow through a channel or pipe is described by de Saint–Venant

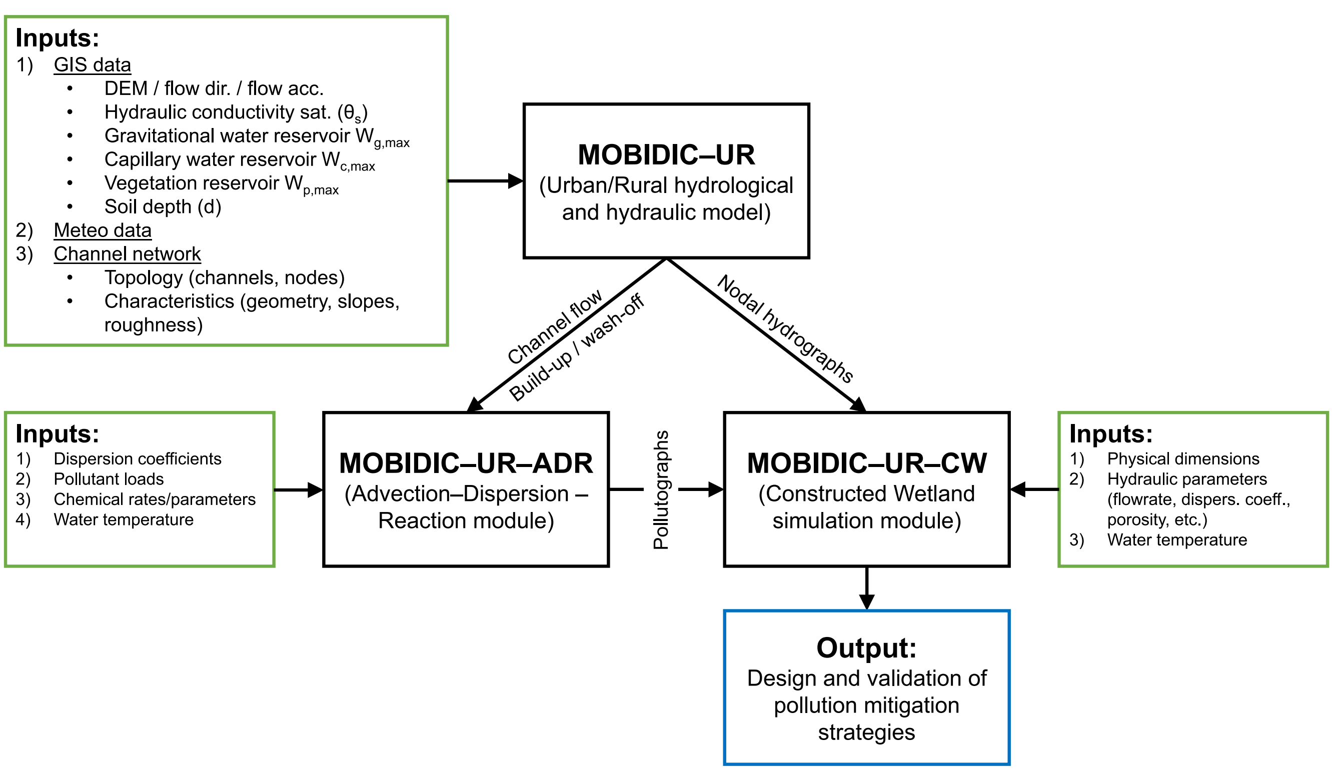

Fig. 1. Structure of the modelling framework. Blocks with green frames show the required model inputs and parameters, black frames indicate the software main modules, and the blue frame highlights the final output.

equations which are solved in one-dimensional form by the dynamic wave flow routing method. For a detailed description of the numerical approach see James & Rossman (2010). Accordingly, the computational input required by the hydraulic module of MOBIDIC–UR consists of two GIS layers. The first layer is a polyline-type shape file representing the conduits which includes the following attributes: geometrical characteristics of the cross-section, reach length, roughness, and the topological connections with the network nodes. The second layer is a point-type shape file representing the nodes of the network (i.e., the interconnection between the network links) and its attributes include: the bottom and top elevation (in case of a manhole). Although potentially able to run continuous simulations over long periods, MOBIDIC–UR is specifically designed for event-based runs.

The two modules MOBIDIC–UR–ADR (advection–dispersion–-reaction module) and MOBIDIC–UR–CW (constructed wetland module) developed in this work are described in detail in the following sections.

2.2. Advection–Dispersion–Reaction module (MOBIDIC–UR–ADR)

In this section we describe the implementation of a module capable of simulating the transport of water quality constituent along the network including their reaction kinetics. MOBIDIC–UR–ADR runs decoupled from MOBIDIC–UR, e.g. as a post-processing module. MOBIDIC–UR–ADR can be theoretically coupled to any other hydrodynamic model a-posteriori (e.g., SWMM), as it uses the outputs from the hydraulic simulations (e.g., flow rates, velocities) and uses them as an input for the water quality simulations. Due to this architecture, it is crucial that the time step of the hydrodynamic model is small enough to minimize the coupling errors.

The underlying motivations behind the choice of developing a custom water quality simulation module, instead of making use or coupling with existing models, are listed as follows:

- because the hydrological/hydrodynamic part of the model can be computationally expensive, one goal in transport modelling is to decouple the two models as much as possible;
- most of available software packages for water quality modelling lack of application programming interface (API), therefore they cannot be interfaced with custom-developed code;
- the set of chemical and biochemical reactions can be very specific to the problem to be solved, and model complexity should be adapted according to the availability of data and information on processes occurring in the modelled system;
- the ability to implement custom models to simulate specific problems, such as the constructed wetland treatment processes (MOBIDIC–UR–CW).

Once inside the network, the dissolved constituents are transported within the pipelines or channels. The one-dimensional transport of dissolved constituents along the length of a pipeline (a pipe or channel) is described by the advection–dispersion-reaction equation:

$$\frac{\partial c}{\partial t} = -v\frac{\partial c}{\partial x} + D_L\frac{\partial^2 c}{\partial x^2} + R \tag{1}$$

where c (g m^{-3}) is the concentration of a dissolved constituent, t (s) the time, x (m) the distance, v (m s^{-1}) is the fluid velocity, D_L (m^2 s^{-1}) the longitudinal dispersion coefficient, and R (g m^{-3} s^{-1}) the source/sink term that includes both external sources and chemical and biological reactions. The advection–dispersion–reaction equation (1) is solved for each component in the model.

When reactions are present in the model it is common to decouple the reactive model from the transport model (Zerihun et al., 2005). Decoupling can be obtaining by an operator-splitting procedure which separates the transport equations from the reactive equations (Carrayrou et al., 2004) and solves the problem sequentially. By solving each single problem separately, the numerical methods can be optimized and tailored to the specific set of equations to be numerically solved. From a software implementation perspective, this allows to couple different modules, capable of simulating different physical and chemical processes, with little effort (Barry et al., 1997). To decouple the numerical resolution of advection, dispersion, and reaction we used a sequential non-iterative algorithm (SNIA), which splits Equation (1) into the following system of equations:

$$\begin{cases} \dfrac{\partial \hat{c}_1}{\partial t} + v\dfrac{\partial \hat{c}_1}{\partial x} = 0 \\ \dfrac{\partial \hat{c}_2}{\partial t} = D_L\dfrac{\partial^2 \hat{c}_2}{\partial x^2} \\ \dfrac{\partial \hat{c}_3}{\partial t} = R \end{cases} \tag{2}$$

Advection, dispersion, and reactions are calculated sequentially, taking into account that the initial conditions of each step correspond to the results obtained from the calculation of the previous step (Bahar & Gurarslan, 2018):

$$\begin{aligned} \hat{c}_1(t_n,x) &= c(t_n,x) \\ \hat{c}_2(t_n,x) &= \hat{c}_1(t_{n+1},x) \\ \hat{c}_3(t_n,x) &= \hat{c}_2(t_{n+1},x) \end{aligned} \tag{3}$$

The following generalized semi-empirical relationship was used to compute the longitudinal dispersion coefficient as a function of the hydrodynamic conditions (Antonopoulos et al., 2015):

$$D_L = a(Hu^*)\left(\frac{U}{u^*}\right)^b\left(\frac{w}{H}\right)^c \tag{4}$$

where $u^* = \sqrt{gR_hS_f}$(m s^{-1}) is the friction velocity, g (m s^{-2}) the gravity acceleration, R_h (m) the hydraulic radius, S_f (−) the hydraulic gradient, H (m) is the average water depth in the section, U (m s^{-1}) the average longitudinal velocity, w (m) the section width, a, b and c are the empirical coefficients to relate the generalized formula back to a specific formula. Specific formulas that can be represented by Equation (4) are, e.g., those proposed by Fischer (1975), Liu (1977), and Seo & Cheong (1998). The equation formulated by Parker (1961) was also implemented.

Beside the described implementation, we also implemented a SWMM-like transport model, in order to validate model results through benchmarking. Numerical implementation is described in James & Rossman, 2010. Since SWMM employs a CSTR approach, it does not directly account for transport by dispersion within the model. Although dispersion is not directly incorporated into the model, an “apparent” dispersion arises due to numerical effects, resulting into an apparent dispersion coefficient. This coefficient is solely dependent on the model’s discretization. This equivalent dispersion coefficient can be calculated as (Socolofsky & Jirka, 2005):

$$D_a = \frac{v\Delta x}{2} \tag{5}$$

where D_a (m^2/s) is the “apparent” dispersion coefficient of tanks-in-series model, v (m/s) is flow velocity, and Δx (m) is the length of the reach between two nodal points.

For the purpose of water quality determination, we considered the following constituents and descriptor parameters:

- Dissolved oxygen (DO)
- Carbonaceous biochemical oxygen demand (CBOD)
- Ammonium (NH_4^+)
- Nitrates (NO_3^-)

In developing the water quality model, we preferred to use simple ad hoc models to derive the crucial information with a small number of model parameters, due to the scarcity of specific information on water quality status. For this reason, the adoption of more complex river quality models such as those made available by the U.S. Environmental Protection Agency (e.g., QUAL2E, QUAL2K, WASP, etc.) would not be feasible in this context. Although the mentioned models can simulate a broad range of water quality parameters, including temperature, pH, conductivity, inorganic suspended solids, dissolved oxygen, various forms of carbon, nitrogen, and phosphorus, as well as phytoplankton, detritus, pathogens, alkalinity, total inorganic carbon, and bottom algae characteristics, their extensive data requirements far exceed the available information and the parameters relevant to this context. Therefore, we adopted a simplified water quality model for describing carbon and nitrogen dynamics, proposed by Marsili-Libelli & Giusti (2008). Although both nitrogen and phosphorus influence uptake dynamics and biogeochemical cycles in streams, phosphorus was excluded from the model due to its distinct biogeochemical behavior and relatively low concentrations compared to total nitrogen in the case study. This allowed us to focus on nitrogen as the primary nutrient of interest, which was more relevant to the specific conditions and objectives of the study.

The model equations describing the dynamics of carbon, nitrogen and dissolved oxygen were as follows:

$$\begin{aligned}
\frac{dB}{dt} &= -K_b\,B + B_s \\
\frac{dNH_4^+}{dt} &= -K_a\,\mathrm{NH}_4^+ + \mathrm{NH}_{4,s}^+ \\
\frac{dNO_3^-}{dt} &= K_a\,\mathrm{NH}_4^+ - K_o\mathrm{NO}_3^- + \mathrm{NO}_{3,s}^- \\
\frac{dDO}{dt} &= K_r\,(\mathrm{DO_{sat}} - \mathrm{DO}) - K_b\,B - 4.57\,K_a\,\mathrm{NH}_4^+
\end{aligned} \tag{6}$$

where B (g m^{-3}) is the concentration of CBOD, NH_4^+ (g m^{-3}) the ammonium concentration, NO_3^- (g m^{-3}) the nitrate concentration, B_s, $\mathrm{NH}_{4,s}^+$, $\mathrm{NO}_{3,s}^-$ (g m^{-3} s^{-1}) represent the sources of CBOD, ammonium and nitrate respectively, K_b (s^{-1}) the kinetic constant for CBOD degradation, K_a (s^{-1}) the kinetic constant of nitrification, K_o (s^{-1}) the kinetic constant of denitrification, K_r (s^{-1}) the reaeration coefficient, DO (g m^{-3}) the concentration of dissolved oxygen, and $\mathrm{DO_{sat}}$ (g m^{-3}) the saturation concentration of dissolved oxygen. All reactions were assumed to be first-order. The concentration of dissolved oxygen at saturation as a function of the temperature was calculated with the following equation (Elmore and Hayes, 1960):

$$\mathrm{DO_{sat}} = 14.652 - 0.41022T + 0.0079910T^2 - 0.000077774T^3 \tag{7}$$

where T (°C) is the water temperature.

The reaeration coefficient K_r (s^{-1}) was estimated with the following generalized empirical formula, as a function of water velocity, turbulence, and water head (S. C. Chapra, 2008):

$$K_c = \alpha u^\beta H^{-\gamma} \tag{8}$$

where K_c is expressed in day^{-1}, H (m) is the average water depth, α, β, and γ are empirical coefficients.

The CBOD degradation constant was calculated as a function of water head with the following equation (Thomann & Mueller, 1987):

$$K_b = \begin{cases} 0.0125\left(\dfrac{H}{2.4384}\right)^{-0.434} & 0 \leqslant H \leqslant 2.4\,\mathrm{m} \\ 0.0125\,H^{-1} & H > 2.4\,\mathrm{m} \end{cases} \tag{9}$$

The temperature dependence of the kinetic constants was calculated with the Arrhenius equation (S. C. Chapra, 2008):

$$K(T) = K(T_0)\theta^{(T-T_0)} \tag{10}$$

where T_0 is the reference temperature (20 °C). We assumed θ = 1.047 for CBOD (K_b), θ = 1.024 for K_r, and θ = 1.07 for K_a and K_o.

Finally, to include the effect of dissolved oxygen concentration on degradation, nitrification and denitrification kinetics, an inhibition factor was introduced for each of the three processes. We used the exponential formulation (S. Chapra & Pelletier, 2003):

$$\left.\begin{aligned} K_{b,i} &= f_b\,K_b \\ f_b &= 1 - e^{-K_{\mathrm{bin}}\cdot \mathrm{DO}} \end{aligned}\right\}\ \text{Biodegradation} \tag{11}$$

$$\left.\begin{aligned} K_{a,i} &= f_a\,K_a \\ f_a &= 1 - e^{-K_{\mathrm{ain}}\cdot \mathrm{DO}} \end{aligned}\right\}\ \text{Nitrification} \tag{12}$$

$$\left.\begin{aligned} K_{d,i} &= (1-f_d)\,K_d \\ f_d &= 1 - e^{-K_{\mathrm{din}}\cdot \mathrm{DO}} \end{aligned}\right\}\ \text{Denitrification} \tag{13}$$

In applying the quality model, some simplifying assumptions were made for modelling CBOD and nitrogen:

- For event-scale simulations, the effects of submerged vegetation (reduced photosynthetic activity due to reduced solar radiation because of increased turbidity) can be neglected.
- The sedimentation of CBOD and nitrogen associated to particulate matter can be neglected, assuming that CBOD and N are mainly related to the fine fraction that remains in suspension, under the simulation conditions.
- Resuspension of CBOD and N from the bottom sediment is neglected. It is assumed that the fine component is always in suspension during the event and therefore resuspension only affects the coarser component.
- It is assumed as a first approximation that CBOD and N are 100 % in dissolved (hydrolysed) form.

The computational effort for solving the full transport Equation (1) is significantly higher compared to a simplified approaches such as CSTR approximation used in SWMM. Therefore, the selection of numerical methods for integration of the transport equation is crucial. Conventional Eulerian methods requires that the dimensionless 'Courant number' Cr to be small enough in order to achieve stability of the numerical solution. However, due to the variability of the flow conditions in the network, these methods are often unsuitable (Croucher & O'Sullivan, 1998). Pure advection problems can be solved with Lagrangian-based method, which are accurate and stable regardless of the Cr number. However, Lagrangian approach requires a moving grid where the nodes of the grid move with the flow. We used a mixed Eulerian–Lagrangian method that combines high accuracy of Lagrangian methods and the simplicity of a fixed Eulerian grid (Bell & Binning, 2004).

The formulation of the entire problem through operator-splitting, as expressed by Equation (2), allowed us to choose different solvers for each subproblem. A semi-Lagrangian method (Bahar & Gurarslan, 2018) in conjunction with a cubic spline interpolation scheme (Ahmad & Kothyari, 2001) was used for numerically solving the advection transport equation. This method has been shown to be quite accurate and stable (Schohl and Holly, 1991). Compared to Eulerian scheme, which has a Courant number restriction on the time-step size for its stability, the adopted scheme has no theoretical limitation on the size of the time step (Socolofsky & Jirka, 2005). However, time step size should be carefully evaluated to avoid errors in the conservation of mass (Fletcher, 2019).

The numerical solution of dispersion equation was achieved through the Saul'yev scheme (Soheili & Arezoomandan, 2013), an alternating-direction finite-difference scheme. It is an explicit method in which computations are performed proceeding in alternating directions, e.g., from left to right and then from right to left of the 1D domain. The method has been shown to be unconditionally stable when integrating from left to right, and conditionally stable from right to left. Stability conditions are discussed by Campbell & Yin (2007).

The mathematical representation of Equation (6) results in a system of ordinary differential equations (ODEs) whose solution was obtained numerically with either ode45 or ode23s solvers, depending on the specific case, available in MATLAB.

The model was applied to the network of channels and pipes coupled with the following mass balance equation for constituent concentrations which is imposed at each node j of the network. For junction nodes that have no storage volume associated, the instantaneous concentration was calculated as:

$$c_j = \frac{\sum_i Q_{i,\mathrm{in}} c_i + F_{\mathrm{in}}}{\sum_k Q_{k,\mathrm{out}}} \tag{14}$$

where c_j (g m^{-3}) is the instantaneous concentration of one species in the j-th node, $Q_{i,\mathrm{in}}$ (m^3 s^{-1}) is the flow rate into the j-th node from the i-th link, c_i (g m^{-3}) the concentration at the end on the i-th inflow link, F_{in} (g s^{-1}) is the mass flow rate of the constituent into the node (i.e., a direct external source), and $Q_{k,\mathrm{out}}$ (m^3 s^{-1}) is the flow rate from the j-th node to the k-th outlet link. The concentration c_j was taken as a Dirichlet boundary condition for the integration of the transport equation at each time step.

2.3. Constructed-Wetland module (MOBIDIC–UR–CW)

Our approach to constructing a Constructed Wetland (CW) model focused primarily on determining the optimal size of these systems to treat influent with specified characteristics, rather than replicating the processes of an actual treatment system. Detailed simulation would require data specifically collected for model calibration and validation. Therefore, we opted to combine a simplified flow and transport model with the more complex and widely accepted Constructed Wetland Model No1 (CWM1) developed by Langergraber et al. (2009). The CWM1 serves as a reference model for biochemical transformation and degradation processes in subsurface flow constructed wetlands. The full

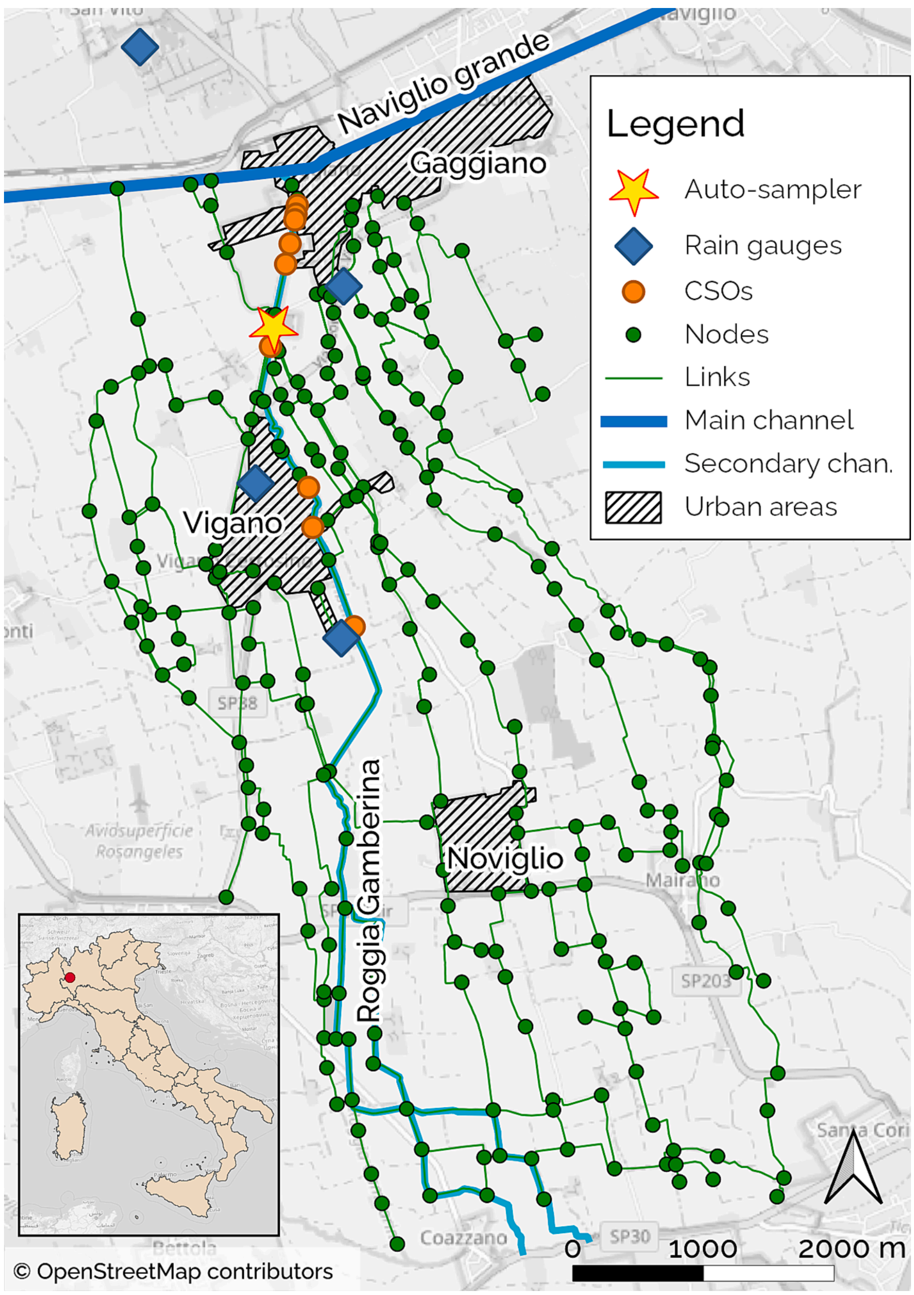

Fig. 2. Network topology of the hydrographic system in the municipality of Gaggiano, Italy.

formulation of the CWM1 model and suggested parameters are described by Langergraber et al. (2009). We implemented the CWM1 in the MATLAB environment, similar to the implementation of the reactive model in MOBIDIC–UR–ADR described in the previous paragraph.

Several approaches have been tested for describing the hydraulic flow. Marsili-Libelli & Checchi (2005) used a combination of series/parallel CSTR models. Giraldi et al. (2010) used the Richards' equation for describing the unsaturated water flow in vertical flow constructed wetlands; Jang et al. (2018) used an unsaturated flow model as well, which they applied to HFCWs.

We chose to couple the CWM1 with a simplified version of the model developed by Boog et al. (2019). Specifically, we implemented a one-dimensional saturated flow and transport model similar to that described for the MOBIDIC–UR–ADR module, with the distinction that the dispersion coefficient pertains to the mechanism of longitudinal dispersion in a porous medium.

2.4. Case study

The MOBIDIC–UR model framework was applied to the hydrographic system in the municipality of Gaggiano (Milan, Italy) to simulate the hydraulic behaviour and water quality of the channel network in relation to specific hydrological events. The study area, shown in Fig. 2, has an extent approximately 6 x 8 km and it is located within a rural area southwest of the metropolitan city of Milan. It comprises a main channel, Naviglio Grande, which delimits the northern boundary of the study area. The major channel in the study domain, referred to as "secondary channel" in Fig. 2, is the Roggia Gamberina, a rural canal of a mixed character, i.e., which receives an inflow from Naviglio Grande and distributes water for irrigation. It also receives drainage water from a series of CSOs from the drainage network of the towns of Gaggiano and Vigano.

In the study domain there are three main areas with different characteristics: an urban area, an industrial area and a prevailing agricultural area. The urban area of Gaggiano is about 2.5 km^2 with a population of about 10,000 inhabitants. The industrial settlement in Vigano, is separate from the urban area and it is located downstream from Gaggiano. The latter has an extent of about 0.5 km^2 and is characterized by industrial buildings mainly for logistics and transportation services. Another smaller urban area is located further south, Noviglio, which has an area of about 0.5 km^2. The drainage network of the municipality's sewage system is of a mixed type, that is, capable of receiving both drainage water from impermeable surfaces and wastewater from civil and industrial sources. Finally, the agricultural area is mainly cultivated with rice, irrigated with a submergence technique from April to September.

Three permanent rain gauges are installed in the study area. They are owned by the water service operator of the metropolitan city of Milan (Cap Group), having a measurement frequency of 1 min and thus capable of detecting in detail even the evolution of short-duration event. Additionally, one automatic water quality sampling station was temporarily installed in the area. The water quality automatic sampler (P6 Mini, Maxx Industry) was placed downstream of the last overflow point that drains surplus water from the urban area into the Roggia Gamberina. The sampler consisted of a 24-bottle canister, and a differentiated acquisition sequence was set for three sets of 8 bottles. The measurements were triggered during rainfall events. After the measurement started, the first 8 bottles were sampled with a 5 min interval, the second 8 with a 15 min interval and the last 8 with a 30 min interval. On each water sample, the following chemical and physical parameters were evaluated: COD, total nitrogen, total phosphorus, metals (Al, As, Cd, Cr, Fe, Mn, Ni, Pb). At the same location, a radar level sensor (Vegaplus C11, Vega) was installed to continuously monitor the water levels. A flow rate scale was appropriately calibrated at the study site to obtain the values of flow rates from the water heights. More detailed information on the sampling campaign is reported by Niazkar et al. (2024).

The topology of the network (Fig. 2) was partially obtained from data available for the main channels and was further manually processed for increasing the level of details and for topological error correction. The network consisted of 291 links and 255 nodes. Links had a width in the range 1.6 to 10 m, and 4 m average. The minimum and average link length was 25 m and 1253 m respectively, for a total of about 105 km. Channel slopes were in the range 0 to 2 % with an average of 2 ‰. Spillways (CSOs) in the urban areas of the domain (Gaggiano and Vigano) interconnected with the rural network have been integrated into the network. Most of them are located along the channel Roggia Gamberina.

2.5. Case study: Model setup

The properties of soils required for the hydrological simulation (i.e., the maximum storage of the gravitational reservoir $W_{g,max}$ and the maximum storage of the capillary reservoir $W_{c,max}$; notation can be found in Yang et al., 2014) were calculated from two main datasets:

- 3D Soil Hydraulic Database (EU-SoilHydroGrids version 1.0) of Europe at 250 m resolution (Tóth et al., 2017), which contains information on the hydrological characteristics of soils at different depths (water content at saturation, hydraulic conductivity, and water content at field capacity).
- Pedology of the soils of the Lombardy Region, at the 250 k scale. Data available from the Lombardy Region Catalog ("Geoportale della Regione Lombardia").

The other parameters of the hydrological model, i.e., percolation coefficient (γ), adsorption coefficient (κ), hypodermic flow coefficient (β), and hillslope flow coefficient (α) were selected based on a previous study conducted on a nearby area (Ercolani et al., 2018), as follows: $\gamma = 1 \times 10^{-5}\ s^{-1}$, $\kappa = 1.8 \times 10^{-6}\ s^{-1}$, $\beta = 8 \times 10^{-5}\ s^{-1}$, $\alpha = 2 \times 10^{-3}\ s^{-1}$.

In addition to the discussed parameters, the hydrological module required the raster of directions and accumulations which were calculated from the DEM (source: LiDAR data – Regione Lombardia, at 1 m resolution). Being a flat area, we could not directly use the terrain DEM to perform hydrological analysis, therefore a modified DEM was purposely constructed from the node elevations by identifying a spatial region for each node with a proximity-based criterion and extruding the elevation upwards starting from the elevation at each node. The watershed was discretized with a spatial resolution of 5 m. The GIS data used are shown in Fig. 3.

The modelling of rural areas is particularly critical due to poor availability of data, in particular those related to the morphological characteristics of the network. For the hydraulic simulations with MOBIDIC–UR the following parameters were also required: (i) cross-sectional geometry of channels, (ii) node elevations, (iii) width of the sections, (iv) Manning's roughness coefficients. With the exception of main channels, such information was not readily available. To address this, we developed an algorithm that automatically extracted the section elevations and geometries were extracted from the DEM. To extract the cross-sectional profiles, the algorithm subdivided the link into multiple sublinks, from which cross sections were extracted and their profiles are derived through interpolation of the DEM. Subsequently, the algorithm automatically determined the geometric characteristics of the sections, such as width and height, through a series of operations: point interpolation and smoothing, identification of the channel bottom (closest to the centerline), delineation of the entire channel bottom plateau, and recognition of the banks. The identified cross sections were then simplified into trapezoidal geometries. Examples of automatically identified cross-sectional geometries are shown in Fig. 4.

Afterward, the algorithm automatically computed node elevations from the DEM. To reduce estimation errors, rather than extracting the single-point elevation at the node location, which may be compromised

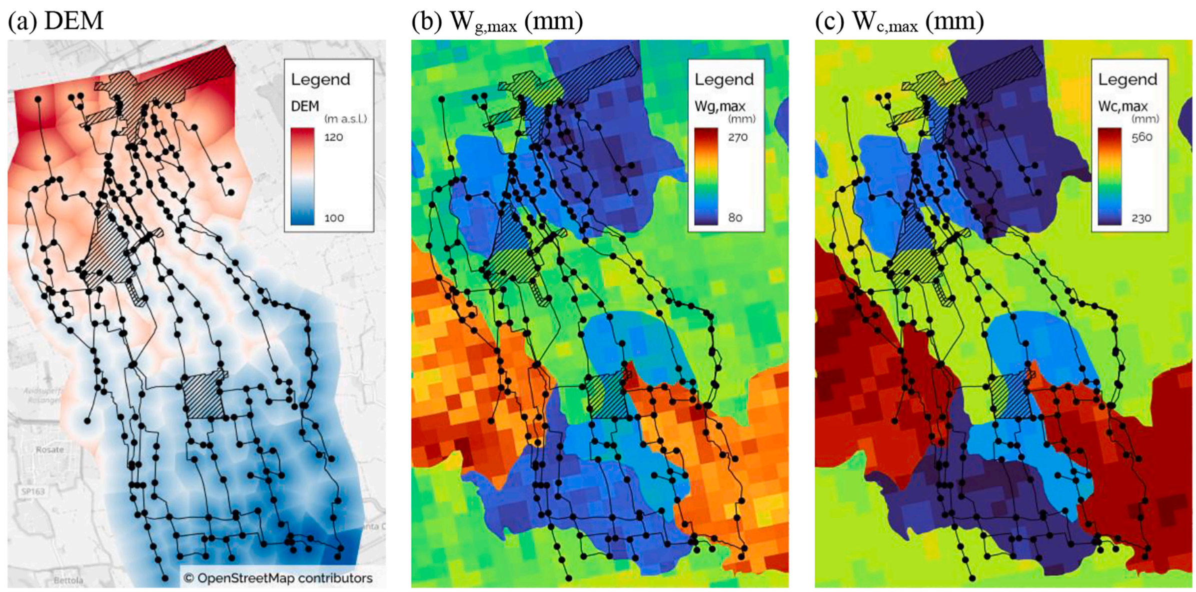

Fig. 3. Hydrological properties in the study domain.

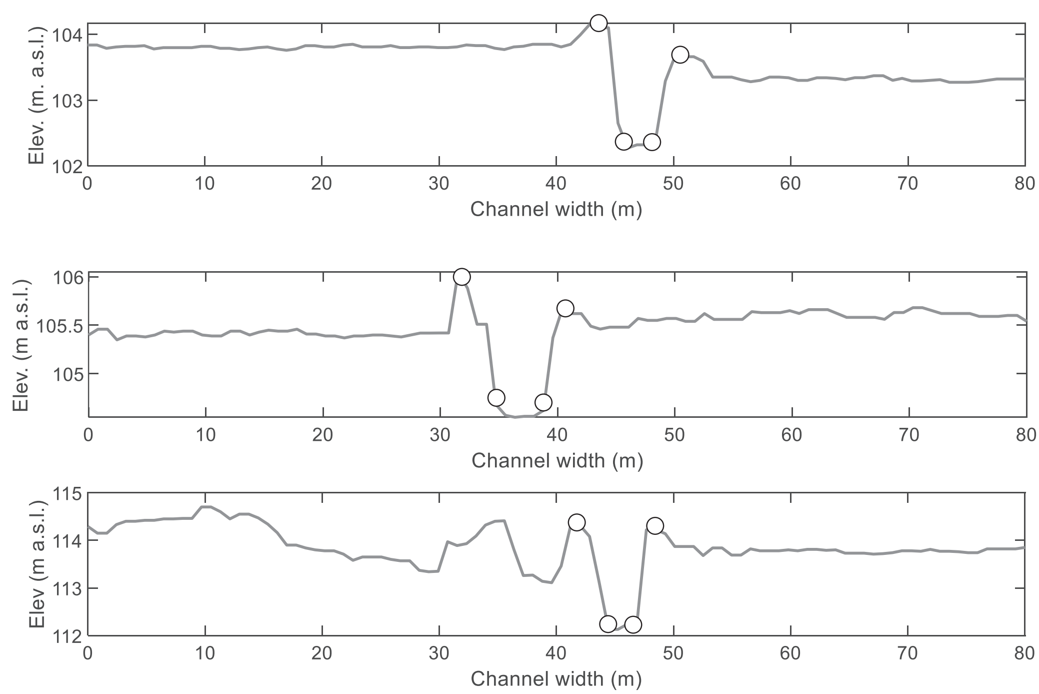

Fig. 4. Examples of automatically identified cross-sectional geometries.

by DEM inaccuracies or misplaced nodes, the algorithm statistically determined the elevation through the following steps: creating a buffer of radius R centred on the node, evaluating the first N samples of the DEM at the lowest elevations, and removing any outliers.

For the selection of Manning's coefficients, 0.02 s $m^{-1/3}$ was assigned to all channels. This value represented an average between the two most common bottom materials (i.e., earth and concrete), both exhibiting similar characteristics regarding vegetation presence. For all MOBIDIC–UR simulations, the hydrological time step was set to 5 min, while the flow routing through conduits in the network was computed with sub-steps of 3 s.

The MOBIDIC–UR–ADR water quality module was setup with a coupling time step between advection, dispersion and chemical reactions of 30 s. The following water quality constituents were included in the model: dissolved oxygen (DO), carbonaceous biochemical oxygen demand (CBOD), ammonium (NH_4^+), and nitrates (NO_3^-). A non-reactive component was included in the model to calculate the mass balance error. The mass balance error was quantified by calculating the percentage difference between the total mass entering in the system and the mass leaving the network at the outlet nodes. To transform the measured quantities into the model variables we used the following relationships:

- COD/CBOD = 2.0
- The relationship $N = NH_4^+ + NO_3^- + NO_2^- +$ organic nitrogen was used to derive NO_3^- values, assuming negligible NO_2^- and organic nitrogen concentrations.

The parameter values for the biochemical reactions implemented in

MOBIDIC–UR–ADR are adopted from Marsili-Libelli & Giusti (2008) and summarized in Table 1.

The last parameter that is needed as input to the model is the dispersion coefficient, which is crucial to estimate because its values can vary widely, often spanning several orders of magnitude. This coefficient typically constitutes a major source of uncertainty in pollutant transport models. A specific study was conducted to determine the dispersion coefficient from field measurements in the case study area (Peruzzi et al., 2021). The results indicated that the formula developed by Parker (1961) provided the most accurate estimates. This study allowed us to reliably estimate the dispersion coefficient under the hydrodynamic conditions analyzed.

The application of the MOBIDIC–UR–CW model was off–line with respect to the other two modules MOBIDIC–UR and MOBIDIC–UR–ADR, as there was no loop from the results of the constructed wetland simulations back to the hydrodynamic and water quality software modules. In implementing a treatment system by horizontal flow constructed wetland, we assumed that a water volume could be withdrawn from one channel, to be conveyed to the wetland. The treatment scheme is shown in Fig. 5.

The treatment system consisted of an initial storage tank for homogenization of pollutants and a treatment basin with size (i.e., length, cross-sectional width and depth) compatible for the implementation of the wetland located in the investigated area.

To transform the concentrations from MOBIDIC–UR–ADR state variables (i.e., CBOD, $NH_4^+ + NO_3^-$, DO) to MOBIDIC–UR–CW (i.e., 19 input variables of CWM1 model) and vice versa, the influent was fractioned according to Mburu et al. (2012). The influent composition was assumed to be comparable to urban wastewater since the contamination primarily originated from combined sewer overflow (CSO) discharges. Consequently, the selected COD fractionation ratios were based on the standard values provided by the Activated Sludge Models (ASMs), which constitutes the foundation of the CWM1 model, i.e., S_a (acetate) = 0.1•COD, S_I (inert soluble COD) = 0.04•COD, X_S (slowly biodegradable particulate COD) = 0.61•COD, and S_F (fermentable, readily biodegradable soluble COD) = 0.25•COD. X_I (inert particulate COD) initial concentration and all initial bacteria concentrations were set to 0.01 gm^{-3}. S_{H2S} (dihydrogensulphide sulphur) and S_{SO4} (sulphate sulphur) were assumed not to be present in the influent.

3. Results

3.1. Model benchmarks

The developed modeling framework was validated by comparing its results with those obtained from other software. Two benchmarks were conducted to validate the MOBIDIC–UR–ADR module: the first benchmark validated the advection–dispersion-reaction code under steady-state flow conditions, while the second benchmark verified both the coupling of unsteady flow simulations in MOBIDIC–UR and the reactive transport calculations in MOBIDIC–UR–ADR. Additionally, two benchmarks were performed to validate the MOBIDIC–UR–CW module: one focused on hydraulic simulations, and the other on biogeochemical reactions. Details are reported in the Supplementary Material document.

Table 1
MOBIDIC–UR–ADR parameters for biochemical reactions.

Parameter	Description	Value	Units
K_b	CBOD decay coefficient	1	day^{-1}
K_{bin}	CBOD inhibition coefficient	0.6	$m^3\ g^{-1}$
K_a	Nitrification rate	0.5	day^{-1}
K_{ain}	Nitrification inhibition coefficient	0.6	$m^3\ g^{-1}$
K_d	Denitrification rate	0.139	day^{-1}
K_{din}	Denitrification inhibition coefficient	0.6	$m^3\ g^{-1}$
α	Reaeration equation coefficient	1	–
β	Reaeration equation coefficient	0.8	–
γ	Reaeration equation coefficient	2	–

3.2. Case study: Numerical simulations

Three rainfall events occurred on 29 April 2021, 1 May 2021 and 4 July 2021, respectively, were simulated on the Gaggiano study domain. The event of 1 May was used as a reference case to calibrate the hydrological model. Only one parameter was adjusted for calibration, i.e., the saturated hydraulic conductivity, which was tuned to 2.8×10^{-8} m s^{-1} for the urban and industrial areas and 4.2×10^{-7} m s^{-1} for rural areas. The simulations of the other two events occurred on 29 April and 4 July were performed to validate the hydrologic and hydraulic model.

Since the channel Roggia Gamberina receives a water inflow from the main channel Naviglio Grande, the measured flow rate baseline value prior to the rainfall event was used to infer the inflows to be set as boundary conditions at the nodes connecting the Naviglio Grande to the simulated network.

Fig. 6 compares the measured and simulated hydrographs that occurred in Roggia Gamberina during the three rainfall events of 1 May (used as calibration event) and 29 April and 4 July 2021 (used as validation events). Measured and simulated data refers to the section where the auto-sampler and level meters were installed (see Fig. 1). The model performance was evaluated using root–mean–square error (RMSE) and Nash–Sutcliffe efficiency (NSE) coefficient (Nash & Sutcliffe, 1970). The latter is widely used in literature for evaluating the quality of predictions of hydrological models. Model performances are reported in Fig. 6. Both RMSE and NSE metrics depict a high level of performance of the model for all three simulated events. The NSE metric is highest for the calibration event (1 May). The NSE coefficients are slightly lower for the validation events of 29 April and 4 July, however, the overall shapes of the hydrographs and volumes are preserved. The good results obtained for validation events show that the model worked well for events of different magnitude, i.e., peak flow rates for the two validation events are about 1.6 m^3/s and 8.7 m^3/s, respectively. The results for the events of 1 May and 4 July also show that the model was capable of describing hydrologic and hydraulic responses accurately even when triggered by more complex rainfall events, i.e., with multiple peaks and longer durations.

Simulation results for the entire network for the event of 1 May are shown in Fig. 7. In the first stage of the rainfall event, the network initially collected lumped runoff from urban areas (e.g. mainly from CSOs), and as it moved south it received distributed contributions from rural areas. This explains a slight increase in the flow rate gradient from north to south of the study area. Peaks greater than 2 m^3/s were found in various branches of the network up to 2 h after the end of the rainfall event (i.e., from 21:00 to 00:00). For all the simulated events, the network was fully capable of discharging the flow and no floods occurred.

For the water quality modelling exercise, we simulated the event of 1 May. Having only one sampling station data available has driven us to use the measured water quality parameters as input pollutographs (i.e., boundary conditions) for the simulations. This choice was motivated by the fact that the high uncertainty of the location and type of sources over the study area would have led to an ill-posed problem, i.e., too many possible distributions of the sources to be evaluated through a single experimental determination. Another assumption was that most of the pollutants are coming from the CSOs of the main urban area of Gaggiano which is upstream of the sampling station. The contribution of wash-off from agricultural surfaces may be significant, however, our modelling focused on investigating the effect and possible mitigation of the CSO discharges into the rural channels, mainly because agricultural contamination, if present, may be prevented by appropriate policies and sustainable management practices (Lintern et al., 2020). The concentrations of the measured constituents, which were taken as boundary conditions for the water quality simulations, are reported in Table 2. The proposed model relies on measured water quality parameters for

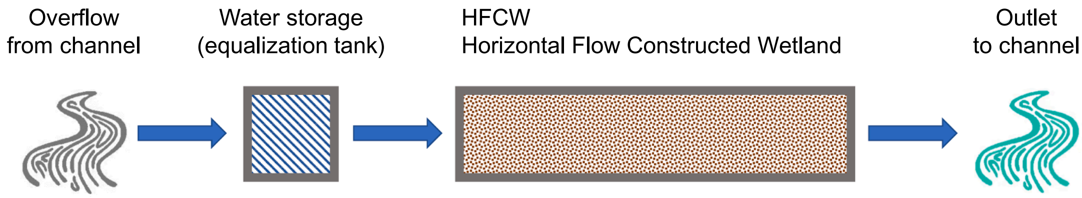

Fig. 5. Horizontal flow constructed wetland (HFCW) treatment scheme.

performing the simulations. Without such data, its direct application is limited. However, users may estimate initial conditions using historical data, empirical relationships, or source-specific assumptions (e.g., pollutant loads from CSO discharge). While these approaches introduce uncertainties, they may provide a basis for preliminary assessments.

The initial concentrations in the model were set to zero for all channels and all constituents, with the exception of dissolved oxygen (DO) which was set to saturation value (about 10 $gO_2\ m^{-3}$) at the water temperature. The water temperature was assumed constant throughout the duration of the event and set to 16 °C.

The simulated period was from 01 May 00:00 to 2 May 23:00. The mass balance error for the non–reactive tracer, included among the components of the model, was 3.75 %. The time evolution of CBOD concentration within the network is shown in Fig. 8. The maps showing the evolution of NH_4^+ and NO_3^- are shown in Fig. S8 and Fig. S9, respectively, which can be found in the Supplementary Material.

The transport of contaminants followed the preferential direction of the flow along the main channel (Roggia Gamberina), with a north to south direction. The simulation revealed that the flow rate from the main channel was rarely transferred to the secondary channels with the exception of a few junctions located west of the town of Noviglio (southernmost urban area) and at the southern end of the network. The CBOD concentration along the Roggia Gamberina got strongly diluted by the runoff and feeds from the secondary channels. Apart from transport along the main channel, the pollutants were conveyed into secondary channels near the town of Noviglio, where their transit was

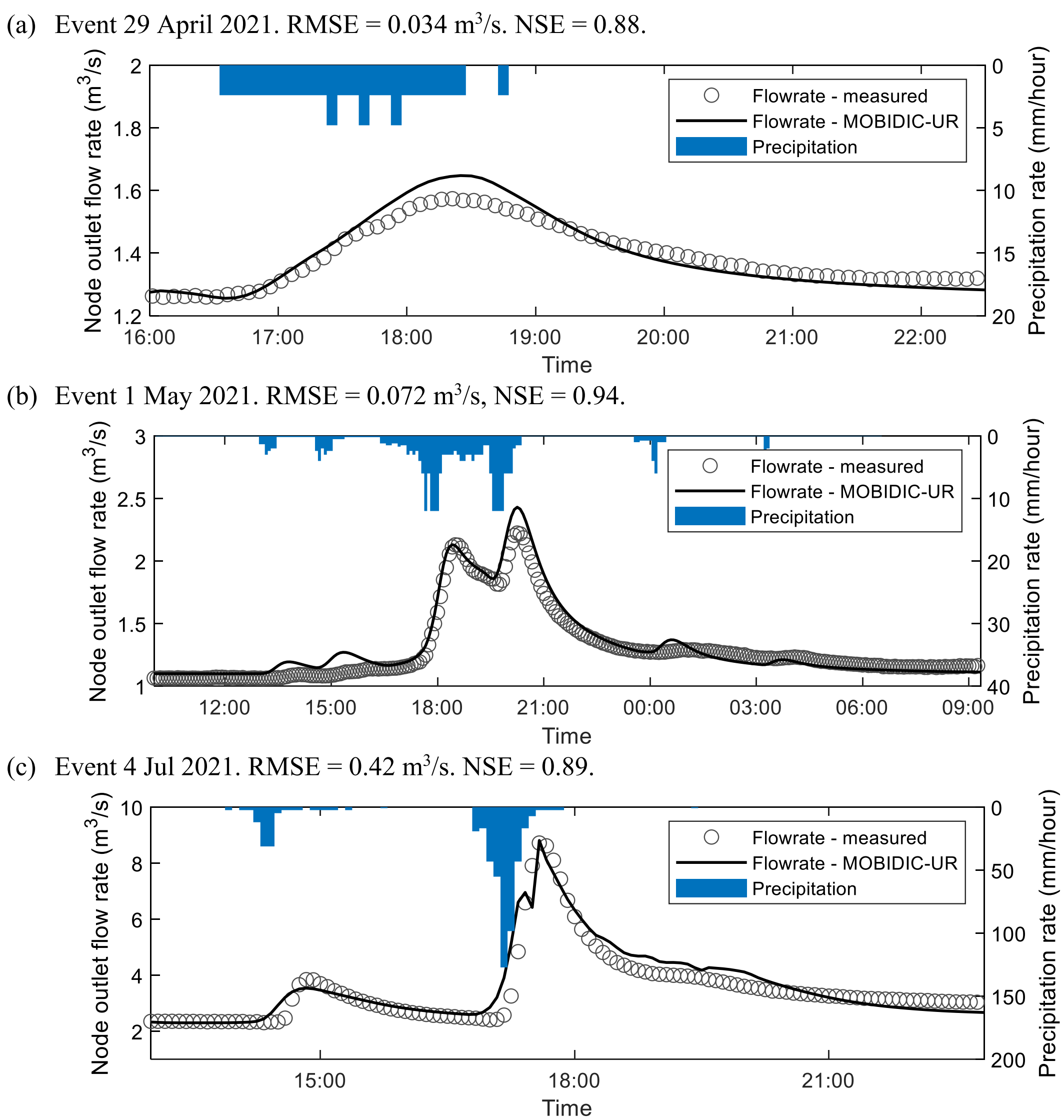

Fig. 6. MOBIDIC–UR simulations for 3 rainfall events occurred on 29 April 2021, 1 May 2021 and 4 July 2021, at the auto-sampler location.

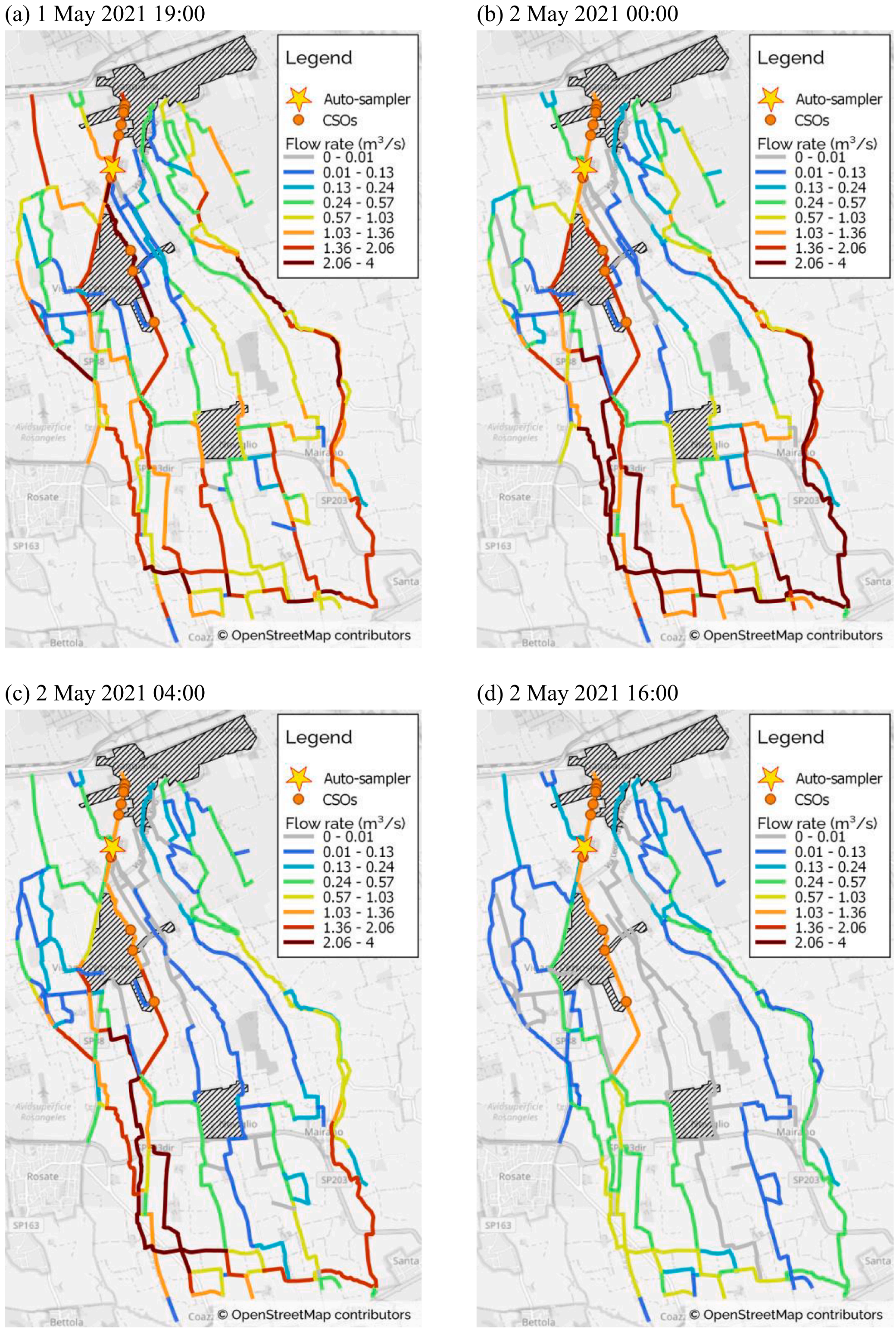

Fig. 7. MOBIDIC–UR flow rate simulations for rainfall event of 1 May 2021.

considerably slower than in the Roggia Gamberina because of slower water velocities. Fig. 8b shows that at 00:00 the CBOD peak in the Roggia Gamberina reached a point further south than the peak in the secondary channel. A high concentration peak occurred located at south of Noviglio with a moderate flow rate and relatively slow velocity. This particular condition and the availability of bare land (currently dedicated to agriculture), led us to select this location to be evaluated as a potential site for the implementation of a horizontal flow constructed wetland to treat pollutant loads from upstream, as will be described in the next paragraph.

The water quality model also allowed us to investigate on the self-purification capacity of the network, by calculating the bulk difference between the total mass entering into the network at the boundary node and the total mass leaving the system at the outlet nodes. The removal by

Table 2
Measured water quality constituent concentrations at the auto-sampler location, event of 1 May 2021.

Date and time	pH	Conductivity (μS/cm)	COD (mg/L O_2	Ammonium (mg/L)	Total nitrogen (mg/L)	Phosphorus (mg/L)	Flow rate (m^3/s)
1/5/21 18:20	9.8	622	438	3.2	13.8	2.4	2.05
1/5/21 18:40	6.9	702	394	2.5	5.9	2.1	2.10
1/5/21 19:00	7	689	250	1	1	1.2	1.92
1/5/21 19:20	6.9	675	172	1	3.3	0.8	1.88
1/5/21 19:40	6.9	688	67	–	–	<0.5	1.81
1/5/21 20:20	6.9	675	95	–	–	<0.5	2.21
1/5/21 21:00	6.9	670	47	–	–	<0.5	1.74
1/5/21 21:40	6.9	666	40	–	–	<0.5	1.50
1/5/21 22:20	6.9	661	20	–	–	<0.5	1.38
1/5/21 23:40	6.9	675	37	–	–	<0.5	1.28
2/5/21 1:00	6.9	676	20	–	–	<0.5	1.29
2/5/21 2:20	6.9	647	20	–	–	<0.5	1.25

biological reactions was 13.7 % for CBOD and 0.41 % for NH_4^+. Conversely, NO_3^- increased by 9.3 %, likely due to nitrification processes. It must be taken into account that this evaluation may be subjected to mass balance errors due to model discretization. As a reference value the mass balance error of 3.75 % for the tracer can be considered. However, taking into account the order of magnitude of the error in the mass balance, one can still conclude that the self–purification capacity was very limited. This is mainly due to the low retention times of water in the channels and indicates that pollutants were mostly transported downstream, leaving the simulation domain.

3.3. *Pollution mitigation: Simulation of constructed wetlands with MOBIDIC–UR–CW*

The water quality simulation results discussed earlier were instrumental in identifying a suitable location for the potential implementation of a treatment system utilizing a non-aerated horizontal flow constructed wetland (HFCW). For siting the HFCW system, the node (Fig. 9) was selected where a peak of CBOD concentration occurred in the secondary channel network. The flowrate and pollutographs were extracted from the selected node to be used as input for MOBIDIC–UR–CW simulation. The diversion of the water volume from the channel was set to be triggered by a minimum CBOD concentration, here taken as > 40 g m^{-3}. When this threshold was exceeded, water started to be withdrawn from the channel. In the present case, the water diversion from the channel into the treatment basin occurred between 1 May 23:15 and 2 May 01:00, with a total volume of about 6264 m^3. The target contaminants to be treated were CBOD, NH_4^+, and NO_3^-.

The performance of the HFCW significantly depends on its design parameters, including the shape, retention time, materials, and aeration. To design the HFCW, we began by considering the available footprint downstream of the selected water diversion node, a space measuring approximately 100 x 150 m, as shown in Fig. 10. This area was designated to accommodate both the equalization basin and the HFCW system. Next, the width and depth of the HFCW were determined using reference values from the literature. For the saturated depth, studies suggest a range of 0.15 to 1.70 m depending on the specific application and local conditions (Pascual et al., 2024). Based on this range, we selected an average depth of 1 m. A width of 3.5 m was chosen, and simulations indicated that a minimum treatment basin length of approximately 1000 m was required to achieve a removal efficiency greater than 80 % for CBOD. To achieve this length in practice, the HFCW can be constructed using a series of meanders, creating a total watercourse of 1000 m. A similar configuration is demonstrated in Lavrnić et al. (2020) for a surface flow constructed wetland located in Northern Italy. An initial hydraulic retention time (HRT) of 4 days, based on recommendations from the literature (Papaevangelou et al., 2016), was chosen as a starting point for the simulations. After evaluation, a final HRT of 2.8 days was selected. A flow rate of 630 m^3 day^{-1} was selected to perform the treatment of the total volume (6264 m^3) in about 10 days. The hydraulic loading rate (HLR) was 18 cm day^{-1}, which falls within the typical range of 2 to 20 cm day^{-1} (D. Q. Zhang et al., 2014). The sizing of the treatment system finally resulted in the parameters reported in Table 3. The table also includes the parameters of the numerical model. The summary of the initial conditions and results of simulations are reported in Table 4. MOBIDIC–UR–CW model outputs are shown in Fig. 10.

Being the HFCW non-aerated, the dissolved oxygen was entirely consumed within about the first 1.5 days of operation (see S_o in Fig. 10a and DO in Fig. 10b). During this initial period the heterotrophic biomass (X_h) growth occurred and caused the biodegradation of S_f (fermentable, readily biodegradable soluble COD) and S_a (fermentation products as acetate). S_{no} (nitrate and nitrite nitrogen) slightly increased after about 1.2–1.7 days of operation due to the nitrification of S_{nh} (ammonium and ammonia nitrogen). Afterwards, S_{no} was consumed due to the denitrification processes. After 2 days the endogenous decay of heterotrophic bacteria (X_h) started, which caused the increase of inert particulate (X_i). After 2 days of operation, due to the low concentrations of dissolved oxygen, the nitrification rate significantly decreased and the concentration of the ammonium (S_{nh}) started to increase.

The removed masses of contaminants after about 10 days of operation for treating the whole volume (6264 m^3) were: 557.9 kg of CBOD, 2.0 kg of NH_4^+, and 17.8 kg of NO_3^-, corresponding to removal percentages of 84.6 % CBOD, 22.7 % NH_4^+, and 83.6 % NO_3^-.

4. Discussion

The model presented here has the potential to be applied in several water management scenario, ranging from urban, suburban, to rural and agricultural settings, where understanding the dynamics of pollution during storm events is crucial for maintaining water quality standards. Its integrated approach, combining hydrological, hydrodynamic, and reactive transport modules, offers a versatile tool for assessing the impacts of various sources of pollution, such as sewerage overflows and runoff from urban and agricultural areas, on the health of receiving water bodies. Due to the diverse sources of pollutants and the complex pathways influencing their behaviour, comprehensive datasets integrating hydrology, climatology, biogeochemistry, and subsurface composition are essential for accurately assessing pollution dynamics. However, such datasets are rarely available (Popp et al., 2024), limiting the practical application of many models. To address this, our approach focused on two key strategies: minimizing the number of model parameters by employing simplified models (e.g., biogeochemical models coupled with transport codes) and prioritizing mechanistic models over empirical or data-driven ones. Mechanistic models like CWM1 rely on parameters widely documented in the literature and accepted as reference values (Langergraber & Šimůnek, 2018)., enhancing their applicability over emerging approaches like machine learning techniques (Tyralis et al., 2019), which often require extensive calibration datasets. Although data collection has significantly improved with the advent of low-cost Internet-of-Things (IoT) sensor networks, these systems primarily focus on monitoring water quantity metrics, such as flow rates

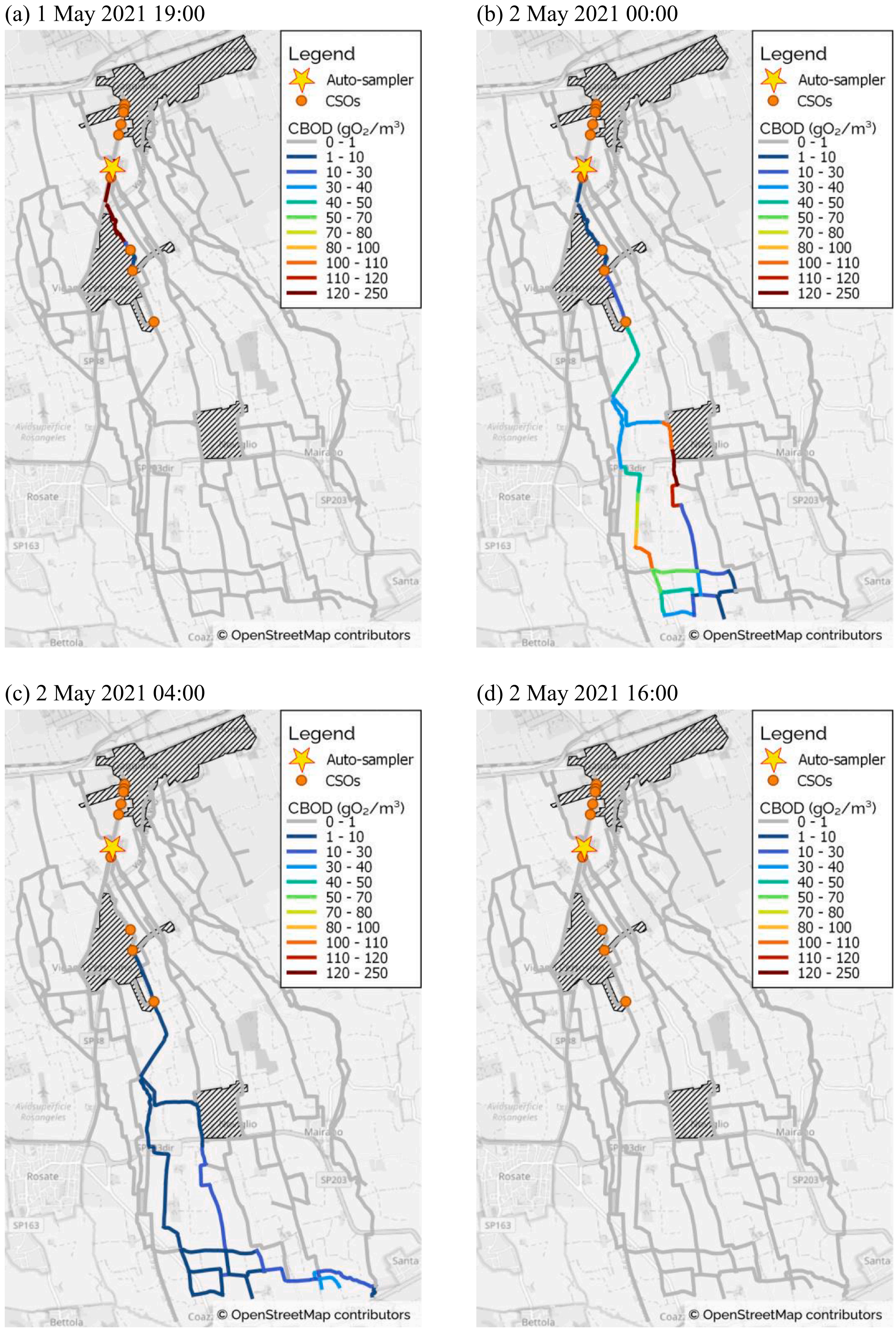

Fig. 8. CBOD simulations for rainfall event of 1 May 2021.

and water depth (Khattar et al., 2023). Real-time water quality monitoring remains a challenge due to the technical limitations of field sensors and the reliance compared to laboratory-based analytical methods for many parameters. This underscores the importance of model designs that can operate effectively even with limited or incomplete datasets.

This modeling approach, designed to function effectively with limited data, is particularly valuable for exploring innovative pollution mitigation strategies in complex urban–rural environments. One possible application of the model is to assess the effect on the reduction of pollutant loads of delocalised treatment areas (CW) with respect to the place of input (CSOs). Since availability of bare land for the implementation of treatment systems is often scarce in urbanised areas, it is possible to exploit the channel network itself to transport water to

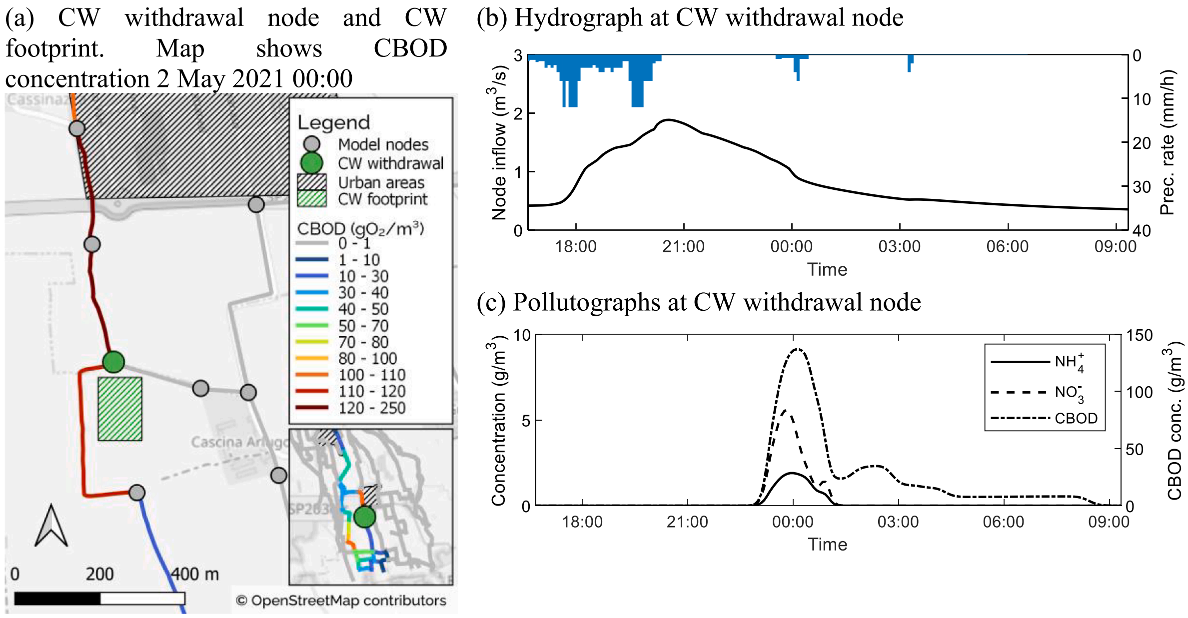

Fig. 9. Node selection as input data for MOBIDIC–UR–CW simulation (a) rainfall event of 1 May 2021, (b) hydrograph, and (c) pollutographs.

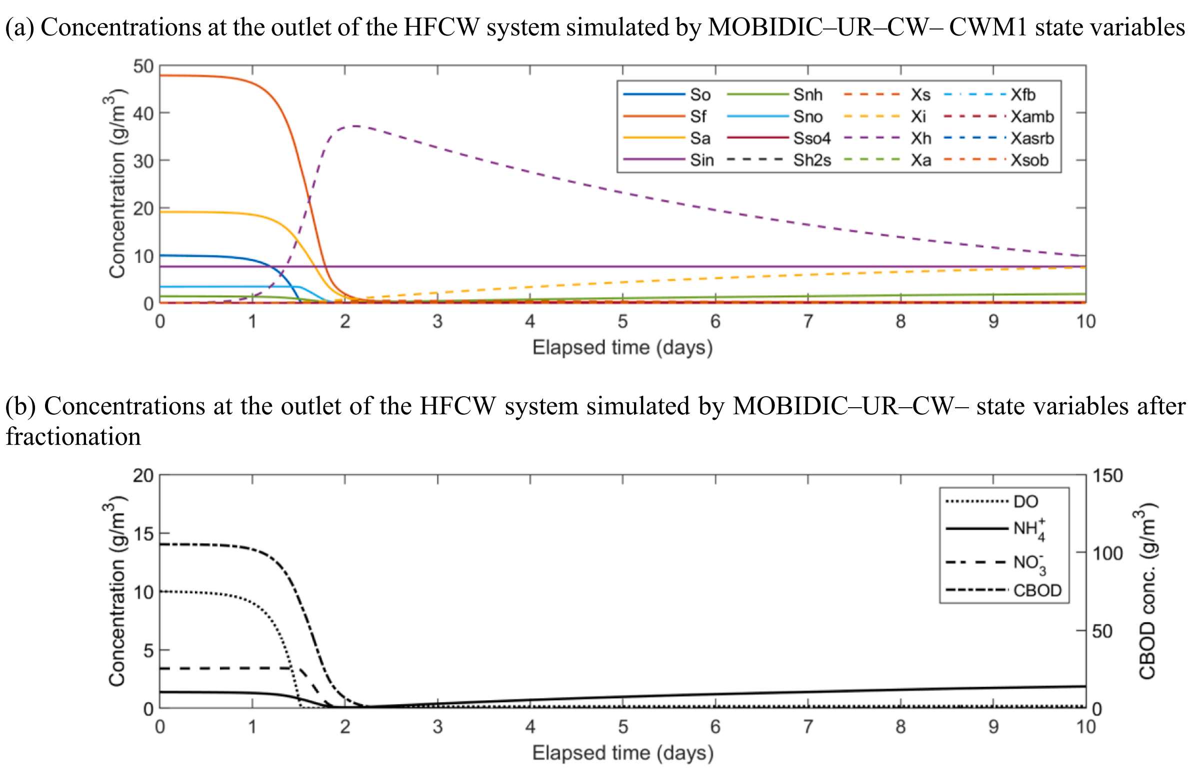

Fig. 10. MOBIDIC–UR–CW simulation results.

locations where it is more convenient to collect and treat the polluted water volumes. The implementation of distributed treatment systems may be particularly relevant for situations where pollution is also distributed spatially, in contrast to cases where pollution occurs at the beginning of the rain event for which first flush tanks may be employed to reduce the impact on receiving water bodies. However, from the measurements carried out in Gaggiano area (Niazkar et al., 2024) and similar cases in literature (Li et al., 2022; Suárez & Puertas, 2005), the first flush does not always occur. In such cases, the MOBIDIC–UR framework can offer a significant support for development and optimization of strategies to mitigate the effects on receiving water bodies. While the effort in this study was focused on the development of a module for simulating the horizontal flow constructed wetlands (MOBIDIC–UR–CW), any other simulation tool can be coupled to MOBIDIC–UR to evaluate other pollution mitigation measures. In the present work, the MOBIDIC–UR–CW software module was instrumental in determining the approximate sizing requirements for the proposed system, designed to manage a rainfall event comparable to that of May 1, 2021. The results we found for the event of May 1, 2021, corresponding to removal percentages of 84.6 % CBOD, 22.7 % NH_4^+, and 83.6 % NO_3^-

Table 3
Constructed wetland characteristics and MOBIDIC–UR–CW parameters for CW simulation.

Parameter	Description	Value	Units
L	Treatment basin length	1000	m
W	Width	3.5	m
d	Saturated depth	1.0	m
n	Porosity	0.4	–
V	Water storage inside the treatment basin	1400	m^3
Q	Flow rate	630	m^3 day^{-1}
HRT	Hydraulic retention time	2.8	days
HLR	Hydraulic loading rate	18	cm day^{-1}
D_L	Dispersion coefficient (porous medium)	1.5×10^{-5}	m^2 s^{-1}
T	Treatment duration	10	days
t	Simulation duration	10	days
dt	Coupling time-step	1200	s
nx	Number of grid points	1000	–

Table 4
MOBIDIC–UR–CW model initial conditions and results summary.

Description	Value	Units
Total treated water volume	6264	m^3
Inlet CBOD concentration	105.2	g m^{-3}
Total inlet CBOD mass	659	kg
Total outlet CBOD mass	101.2	kg
Inlet NH_4^+ concentration	1.4	g m^{-3}
Total inlet NH_4^+ mass	8.7	kg
Total outlet NH_4^+ mass	6.7	kg
Inlet NO_3^- concentration	3.4	g m^{-3}
Total inlet NO_3^- mass	21.3	kg
Total outlet NO_3^- mass	3.5	kg

are consistent with removal efficiencies reported in the literature for subsurface-flow constructed wetlands treating wastewater-like influents, with removal rates of up to 95 % for BOD (Puigagut et al., 2007), and 86 % for total nitrogen (D. Q. Zhang et al., 2014). However, in many of the cases presented in these studies, the average removal efficiencies tend to be lower. The NH_4^+ removal falls within the range of 20 to 54 % among several sub-surface flow CWs reported by (Puigagut et al., 2007). The significantly high variability in the observed removal percentages can be attributed to a range of factors, including the type and characteristic of the treated influent, the specific design of the constructed wetland, climatic conditions, and site-specific operational practices, many of which can only be controlled in-situ.

This analysis offered valuable insights into the system's capacity and efficiency, demonstrating that the proposed HFCW could effectively mitigate pollutant loads under similar conditions.

Although the framework presented offers valuable insights into water quality modelling within the specified context, it is important to acknowledge potential limitations that may arise in its future application: (i) despite efforts to address data scarcity through automated extraction algorithms, there may still be limitations in the availability or accuracy of topological and topographical data, which could affect the precision of model predictions, (ii) improved model validation procedures against observed data should be carried out especially focusing on water quality parameters and with data from real-case implementations of constructed wetlands, (iii) in relation to this, a dedicated study can be conducted to evaluate the model's sensitivity to parameter uncertainty, (iv) build-up, wash-off, and reactive-transport processes occurring within the hydrological cycle have not yet addresses but could be relevant in many scenarios, and (v) larger datasets are needed to assess the relative importance of the interactions between pollutants and sediments and solid transport processes on pollutants transport dynamics. The abovementioned limitations, however, could constitute an important basis upon which future research can be established.

5. Conclusions

We presented a comprehensive numerical model aimed at simulating coupled hydrological, hydrodynamic, and reactive-transport of dissolved chemical species for studying the fate, the effects, and possible mitigation strategies of pollution originated from combined sewerage systems discharging into an interconnected network of receiving waterbodies in a mixed urban–rural environment. The modelling framework comprised three software modules: (i) MOBIDIC–UR, a hydrological and hydrodynamic module capable of simulating run-off and propagation in the channel network, (ii) MOBIDIC–UR–ADR, an advective–dispersive-reactive transport model, and (iii) MOBIDIC–UR–CW, a module designed to asses and size horizontal flow constructed wetlands for pollution mitigation. Given the limited availability of data in rural areas, particularly regarding network morphology, we developed an algorithm to automatically extract topological and topographical data from digital elevation models. To validate the two newly developed software modules, MOBIDIC–UR–ADR and MOBIDIC–UR–CW, four benchmark experiments were performed, which ensured the accuracy and reliability of the software modules across various scenarios and functionalities.

We applied the model to a case study located in a suburban area of Milan, Italy, to evaluate the effects of sewer overflows and runoff on the water quality of the receiving water bodies. Additionally, the model was applied to determine an appropriate size for a water treatment system based on a horizontal flow constructed wetland for pollution management. The results demonstrate that the modeling tools aid in designing and properly siting effective mitigation strategies which are able to significantly reduce pollutant loads and achieve water quality suitable for agricultural and environmental reuse. Despite the acknowledged limitations of the modelling approach, we believe that the developed framework provides a crucial tool for making informed decisions in water resource management and environmental protection. This is particularly relevant in dynamic urban environments where rapid change is a constant factor. The framework not only recognizes but also quantifies the value of nature-based solutions, highlighting their importance in sustainable water management strategies.

Software availability

The software developed in this study is publicly available at the following GitHub repository:

Repository name: MOBIDIC-UR-ADR-Benchmark.

Repository URL: https://github.com/matteomasi/MOBIDIC-UR-ADR-Benchmark.

Access: Open source under the MIT license.

The repository includes source code, instructions, example data, and documentation required to reproduce the results described in this study.

CRediT authorship contribution statement

Matteo Masi: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Conceptualization. **Daniele Masseroni:** Writing – original draft, Resources, Project administration, Funding acquisition, Formal analysis, Data curation. **Fabio Castelli:** Supervision, Project administration, Funding acquisition, Formal analysis.

Declaration of competing interest

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

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jhydrol.2025.133172.

Data availability

The link to the source code is available in the relevant section of the manuscript ("Software availability")

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