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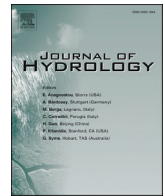
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Research papers

Lumped and semi-distributed modelling for the simulation of flow and water quality in combined sewer networks

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ABSTRACT

The effective environmental management of combined sewer systems requires reliable estimation of discharge and pollutant loads conveyed at the outlet during rainstorms. This study investigates how, with a lumped modelling approach, it is possible to reproduce the quality characteristics of discharged water, provided that high temporal resolution experimental data of pollutant concentrations are available. The methodology is applied to the combined sewer of a real urban drainage network where a continuous high resolution monitoring campaign of water quality and quantity has been carried out at an overflow structure location near the outlet of the drainage system. The lumped modelling approach has been implemented in the Storm Water Management Model (SWMM) with hydrological parameters estimated from cartographic information, based on recently proposed methodology that allows reliably simulating the storm hydrographs without model calibration. A semi-distributed model has been also developed using the SWMM with hydrologic parameters randomly sampled to fit the measured hydrographs of different training and validation data. The results obtained show that the uncalibrated lumped model simulates the observed hydrographs with similar performance as with the semi-distributed model (i.e., the normalized Nash-Sutcliffe efficiency index of the validation set is 0.753 for the uncalibrated lumped model and 0.765 for the best-performing sampled parameter set of the semi-distributed model). The water quality parameters describing the build-up and wash-off of total dissolved solids (TDS) in a lumped model have been calibrated too, as well as those describing the mixing and consumption of dissolved oxygen (DO). The results show that a lumped modelling approach can reproduce the water quality dynamics in a combined sewer system, representing a promising tool for effective environmental management. However, event-specific calibrated parameter values have been obtained in some cases, which require further investigation and still limit the general applicability of the obtained results, thus confirming that setting up a reliable model requires water quality measurements.

1. Introduction

Design, operation, and management of Urban Drainage Systems (UDSs) rely on good modelling practice. A good UDS model should reliably predict hydraulic and water quality parameters in the sewer network under different conditions (Butler et al., 2018), with the purpose of designing and operating the infrastructures, protecting the urban environment from flooding (Piadeh et al., 2022), and avoiding pollution of nearby water bodies due to Combined Sewer Overflows (CSOs) (Petrie, 2021).

Typically, UDS models simulate hydrologic, hydraulic and pollutant release and transport processes (Bach et al., 2014) occurring within the urban catchment. Regarding the hydrological modelling, in literature, approaches with different levels of detail have been adopted (Salvadore et al., 2015; Ji et al., 2025), namely: distributed, in which the variety of hydraulic processes within the drainage system are modelled with physically-based equations (e.g., Pan et al., 2012); semi-distributed, in which the drainage system is represented as a set of sub-catchments, making use of either conceptual and physically based equations (Brendel et al., 2021) or lumped, in which a conceptual model replaces

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the entire drainage system (e.g., Farina et al., 2023).

The aim of the hydrological modelling is to describe the transformation of rainfall in runoff over the catchment surface. The hydraulic quantities in the sewer network are usually calculated solving the Saint-Venant equations (Chow, 1959) for gradually varied unsteady flow conditions. The water quality, instead, is simulated for process understanding, either with empirical or kinetic models, or for predictive purposes, with data-driven approaches such as regression or machine learning models (e.g., Jia et al., 2021). In any case, the aim of water quality modelling is to predict the concentration of pollutants in sewer flows, and thus the assessment of water treatment plant load, as well as potential environmental impact of sewer discharges.

To run any simulation model, the values of its parameters must be determined first. In this respect, model calibration is a common practice (e.g., Gamberth et al., 2011; Muschalla et al., 2008). However, model calibration of UDSs presents several difficulties and uncertainties (Deletic et al., 2012). For example, highly detailed models have many hydrologic, hydraulic and water quality calibration parameters, so that the inverse problem of model calibration may be cumbersome and often lacking uniqueness of solution (Beven, 2006; Okiria et al., 2022; Spear, 1997). This issue can be addressed by using simplified modelling approaches such as surrogate models (e.g., Mahmoodian et al., 2018) or using machine learning approaches (e.g., Li et al., 2023; Garzón et al., 2022). Hydrologic model calibration can be avoided with the lumped approach proposed by Farina et al. (2023), which exploits empirical relationship, based on measured rainfall-runoff transformation in a set of networks with different characteristics, to assign parameters directly from cartographic information.

However, even if the issues of the calibration process were solved, substantial calibration data would still be required to obtain reliable model simulations of water quality. Unfortunately, field experimental data of both water quality and quantity in sewer systems are still very scarce (Moy De Vitry et al., 2019; Pedersen et al., 2021; Vonach et al., 2019), because sewer monitoring is expensive and difficult to manage. Specifically, in literature, water quality monitoring is less common than flow monitoring, due to the high uncertainty in the former (Jia et al., 2021). In studies on water quality in urban environments, wastewater or stormwater sampling techniques are largely more common than continuous monitoring, with limited time resolution of available water quality data (Kim et al., 2022). The lack of water quality data with the temporal resolution required for model calibration, such as those provided by online monitoring sensors (Bertrand-Krajewski et al., 2008; Brzezińska et al., 2016; Métadier and Bertrand-Krajewski, 2012; Schellart et al., 2023), still limits the accuracy of water quality modelling in UDSs (Jia et al., 2021). Consequently, few attempts have been made so far to directly predict the discharged pollutant loads of CSOs (e.g., by Dirckx et al., 2022; Farina et al., 2024; Pistocchi, 2020; Willems, 2006).

As a matter of fact, the regulations aiming at limiting the environmental impact of UDS are becoming increasingly strict (Jensen et al., 2020). Thus, operational modelling tools are needed for their management, in many cases without the help of available measurements of water quantity and quality. While reliable hydrologic modelling of UDS can be carried out with lumped approach without calibration (Farina et al., 2023), setting up general models of water quality is still an issue (e.g., Rodríguez et al., 2013). This is due to the rare availability of suitable experimental datasets of water quality parameters for model calibration (e.g., Popick et al., 2022). Furthermore, established simplified models, with a few unknown parameters, are also lacking, which would make calibration easier.

To contribute to this topic, the suitability of a lumped approach with simplified equations for water quality modelling in a UDS is investigated. Specifically, the case of a real combined UDS is studied, where continuous experimental data of water flow and water quality indicators (namely, dissolved oxygen and total dissolved solids) are available. The data were collected through an online monitoring campaign of surrogate water quality parameters, carried out with a multi-parametric probe at a

CSO near the outlet of the UDS. The experimental data of water flow allowed the calibration of the semi-distributed model of the network in SWMM and the comparison of its simulation performance with that of an uncalibrated lumped model (Farina et al., 2023). The results highlight the issue of identifiability of the many hydrologic parameters characterising the semi-distributed model of the sewer system, even in presence of complete geometric information provided by the local water utility. However, the lumped model satisfactorily reproduced the observed hydrographs without requiring a site-specific calibration and was thus applied also to water quality simulation. The parameters of the relevant equations (i.e., describing mixing processes and build-up and wash-off processes, depending on the considered pollutant) were identified by optimising the goodness of fit between observed and simulated water quality graphs.

2. Methodology

2.1. Overview

In this study, the results of an online monitoring campaign of wastewater and stormwater quality and quantity in a real sewer network are used to assess the suitability of a lumped modelling approach for reliably simulating discharge and concentration of transported species at the outlet of the network. The collected dataset allowed investigating the suitability of a lumped model to hydrologic and water quality simulations. The monitoring campaign started, after a testing period, in September 2021 and ended in July 2023. The recorded data were used to calibrate a semi-distributed model of the urban drainage system of the study site, by optimising the goodness of fitting (GoF) of the hydrographs at the main outlet of the UDS. Furthermore, a simplified lumped model of the system was also applied, with the approach proposed by Farina et al. (2023), that does not need a site-specific calibration of the hydrologic parameters. In this way, only the identification of water quality parameter values required model calibration. With this model, capable of reproducing the observed hydrographs with similar accuracy as the semi-distributed model, simulations of the concentrations of TDS and DO in the outlet were carried out, calibrating the parameters of the water quality equations against the measured concentrations.

2.2. Study area

Urban catchments of densely populated areas are characterised by large fractions of impervious surface (Ramezani et al., 2021), and thus, a potentially high environmental impact of discharges from sewer networks on water bodies (Farina et al., 2024). The densely populated coastal city of Portici, in Italy, was chosen as the study area. Portici belongs to the metropolitan area of Naples, in southern Italy (Fig. 1a), with about 51,000 inhabitants and a population density of nearly 12,000 $\frac{P}{km^2}$ (ISTAT, 2021). The UDS is a combined sewer system and collects wastewater of around 30,000 inhabitants and stormwater from a catchment with area 3.2 km², average slope 3.7 % (altitudes vary between 0 and 144 m above sea level), and 78 % of impervious surface, mostly of it with residential use. The rainfall data are taken from the rain gauge network of the Civil Protection Department (DPCN, 2023a), with ten minutes resolution. In this study, the rainfall data of the rain gauge of Ercolano, 2.7 km east from Portici (Fig. 1b), were used.

The sewer system contains 188 junctions, 189 conduits (in most cases made of reinforced concrete), 5 regulators, 4 overflow structures and a gate valve. The network layout of the sewer system is provided in Fig. 1c. A pumping station, which conveys wastewater and part of the stormwater to a wastewater treatment plant (WTP), is placed downstream the main outlet of the UDS. During extreme storm events, four overflow structures (red dots in Fig. 1c) discharge excess water to the sea, to avoid flooding and WTP overload. One of the overflow structures is located at the main outlet of the UDS (Fig. 1c), where the monitoring

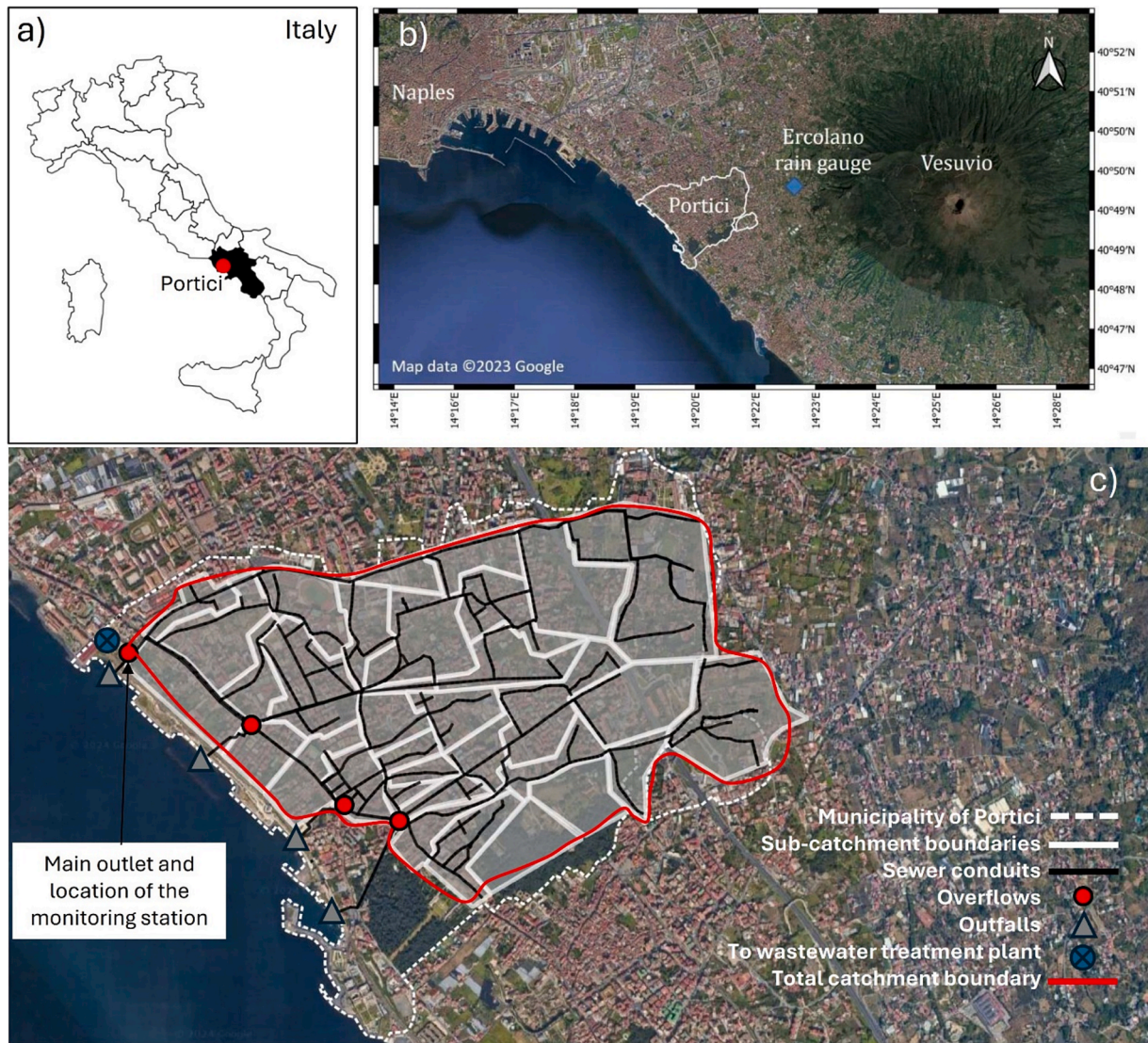


Fig. 1. Location of Portici (Naples) in Italy (a); municipal boundary of Portici and position of the rain gauge of Ercolano, used as rainfall data source (b); layout of the model of the urban drainage system (c).

station was installed.

2.3. Semi-distributed urban drainage model

The semi-distributed (i.e. more detailed) model of the sewer network of Portici was implemented in the Storm Water Management Model (SWMM) (Rossman & Huber, 2016a), relying on Geographic Information System (GIS) data provided by the local water utility, GORI S.p.A, together with established literature recommendations on values of hydrologic parameters of urban catchments. The model consists of a hydrologic and a hydraulic module.

In SWMM, a catchment can be discretised into several sub-catchments, schematised as rectangular inclined planes, with area A , width W (as defined in Rossman & Huber, 2016b), and slope S , subjected to the rainfall intensity i . For each sub-catchment, the runoff from pervious and impervious surfaces is calculated separately, using a nonlinear reservoir conceptual model (Chen & Shubinski, 1971; Rossman & Huber, 2016b), and iteratively solving the following mass conservation and runoff equations:

$$\frac{\partial d}{\partial t} = i - ev - f - q \quad (1)$$

$$q = \frac{W\sqrt{S}}{An}(d - d_s)^{5/3} \quad (2)$$

where i is rainfall intensity, ev evaporation, d is the water depth over the ground and d_s is the height of the depression storages, f is the infiltration rate (for the pervious part only), q is the runoff per unit area, for an equivalent inclined rectangular surface with: slope S , width W , overall area A and Manning roughness coefficient n . To quantify the pervious and impervious parts of the area, the parameter I , i.e. the fraction of impervious surface, is assigned to each sub-catchment. The total runoff from each sub-catchment is the sum of the runoff from both its pervious and impervious parts.

The UDS of Portici was discretised into 33 sub-catchments for the purpose of modelling (represented in Fig. 1c). Sub-catchments were defined based on the location of the sewer network main conduits and on the topographical map of Portici, in turn derived from the digital elevation model of Italy (Tarquini et al., 2023). Variables A , W , and S were retrieved from maps for each sub-catchment. The percentage of impervious surface of each sub-catchment, I , initially evaluated from available maps, was adjusted afterwards based on the comparison between measured and simulated flow. The parameters n and d_s initially set based on literature recommendations (e.g., Chow, 1959; Rossman &

Huber, 2016b), were also adjusted afterwards for the impervious areas. Further details of model parameter assignment are discussed in Section 2.7.

Historical data of rainfall i was available (Section 2.1). Owing to the short duration of the analysed rainstorms ev was neglected, and f was modelled with the modified Horton method (Akan, 1992), such that the pervious areas did not contribute to runoff generation.

To calculate the hydraulic quantities in each channel of the sewer system, SWMM solves the St. Venant equations (conservation of mass and momentum) for unsteady free surface flow through each conduit. The geometric features of each conduit were extracted from the GIS of the network, and the roughness parameters were assigned based on the material of each conduit. Eqs. (1) and (2) and the St. Venant equations were numerically solved with a time discretization interval of 30 s and then resampled to 2 min, so to be consistent with the frequency of acquisition of monitoring data (section 2.5).

2.4. Lumped modelling approach

In a recent study (Farina et al., 2023), a simplified modelling approach to simulate UDSs with little information available and low computational effort was tested against several case studies found in the literature. The approach consisted in assigning few catchment parameters to a simplified lumped model (SM) of the UDS implemented in SWMM. In this approach, the parameters can be assigned a priori from cartographic information, thanks to empirical relationships derived from a set of networks where flow measurements were available. Specifically, the parameters of the lumped model were determined with the following equations (Farina et al., 2023):

$$I_L = 0.51I^{1.2} \quad W_L = 0.87W \quad \frac{W_L \sqrt{S}}{n_L} = 24.28W^{0.8} \quad (3)$$

In Eq. (3), the subscript L denotes the parameters of the lumped model, while the symbols without subscript indicate parameters read from the cartographic information.

The SM showed similar performance, in terms of goodness of fitting of the simulated hydrograph at the outlet section, compared to semi-distributed detailed model (DM), where all the sub-catchments of the urban area are separately described. Besides the reduced computational burden, the SM presents the great advantage of not requiring a site-specific calibration, thanks to the empirical relationships of Eq. (3).

In this study, this approach has been applied to the UDS of Portici

alongside the semi-distributed model. The SM of the UDS of Portici consists of 4 lumped sub-catchments (in place of the 33 of the semi-distributed model), chosen as the upstream catchments of 4 overflow structures of the UDS (Fig. 2). Model parameters assigned based on available cartographic information through the relationships proposed by Farina et al. (2023) and the main characteristics of the four lumped sub-catchments are given in Table 1.

2.5. Water quality simulation model

The transport of pollutants through the conduits is described, assuming complete mixing, with the following simplified mass balance equation (Rossman & Huber, 2016c):

$$\frac{d(Vc)}{dt} = C_{in}Q_{in} - cQ_{out} - VK_1c \quad (4)$$

In Eq. (4), c and V are concentration and volume within the conduit, respectively; C_{in} and Q_{in} represent concentration and discharge of any inflow to the conduit, respectively; Q_{out} is the discharge leaving the conduit; and K_1 is a first-order reaction constant, which can be either assigned based on literature recommendations or calibrated against experimental data of concentration.

A generic compound may be present in the wastewater with an average concentration C_W , and in the stormwater with an average concentration C_R , which are flow weighted averaged:

$$C_{in} = (q_W C_W + q C_R) / (q_W + q) \quad (5)$$

In Eq. (5), q_W represents the dry weather inflow to the conduit. Also, some pollutants may accumulate over the catchment surface during dry weather periods and be washed off during storm events. In this study, to model the water quality dynamics, the build-up (Eq. (6)) and wash-off

Table 1

Main characteristics of the four sub-catchments of the lumped model of the combined sewer network of Portici, and hydrologic parameters estimated with the relationships proposed by Farina et al. (2023).

Catchment nr.	A(ha)	S(%)	W_L (m)	n_L ($m^{-1/3}s$)	d_s (mm)	I_L (%)
1	115.0	3.42	4720	0.0414	1.25	83.9
2	93.4	3.78	2540	0.0384	1.25	98.9
3	27.4	3.12	1428	0.0311	1.25	100.0
4	127.2	4.86	1932	0.0412	1.25	70.7

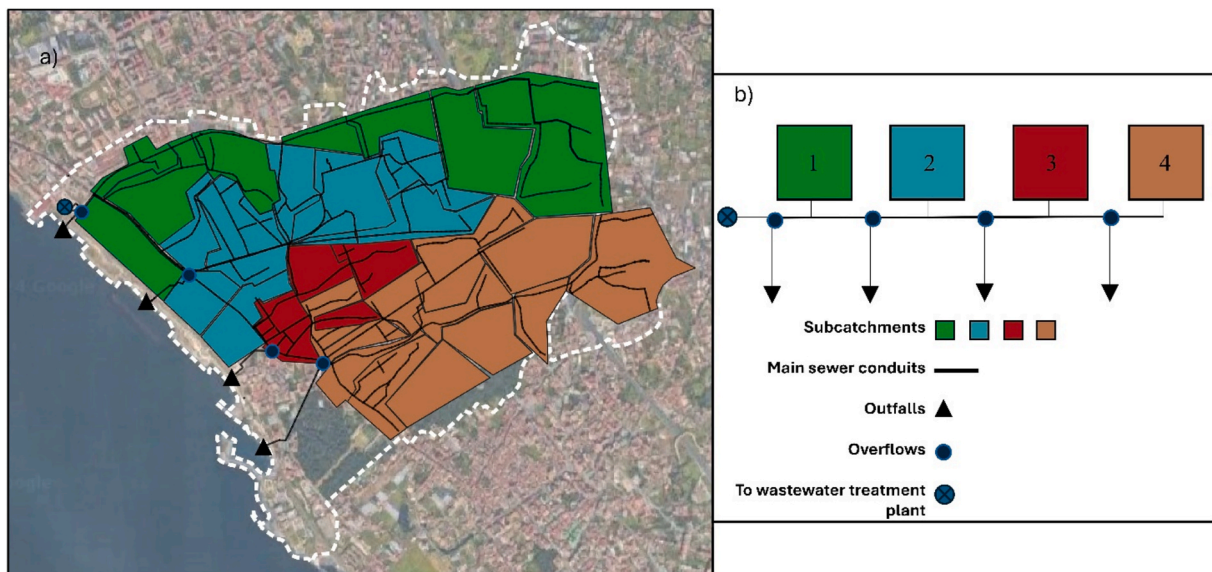


Fig. 2. Scheme of the simplified model of the UDS of Portici, following the approach of Farina et al., 2023.

(Eq. (7)) processes are described by the following exponential equations (Butler et al., 2018; Rossman & Huber, 2016c):

$$b(t_b) = C_1 (1 - e^{-C_2 t_b}) \quad (6)$$

$$w(t_w) = b_0 e^{-C_3 q^{C_4} t_w} \quad (7)$$

where $b(t_b)$ is the mass of pollutant accumulated per unit area, t_b is the antecedent dry weather period, C_1 is the maximum possible accumulation of mass of pollutant per unit area, C_2 is a rate constant; $w(t_w)$ is the pollutant mass per unit area remaining on the ground surface during the wash-off process at the time t_w from the beginning of the rain event, b_0 is the initial mass of pollutant per unit area, C_3 and C_4 are wash-off coefficient and exponent, respectively. The mass rate w can be converted to a concentration by dividing by the runoff per unit area q .

The use of the above-described equations within a lumped model of the sewer network is a novel aspect of the proposed methodology, made possible thanks to the availability of continuous online measurements of water quality parameters and discharge. Specifically, in Eqs. (6) and (7), t_b was known from the rainfall time series, q and t_w were calculated by the hydrologic module, while C_1 , C_2 , C_3 , and C_4 were calibrated, as well as C_R . Differently, as explained in Section 2.6, C_W was in all cases assigned a priori.

2.6. Monitoring campaign

Quality and quantity data of wastewater and stormwater were recorded at the main outlet of the UDS of Portici (see Fig. 1c), continuously, during dry weather and wet weather, with a time resolution of 2 min, at three measurement sections s_1 , s_2 , and s_3 . The experimental dataset spans nearly two years, from September 2021 to June 2023, thus representing a still uncommon source of information on the behaviour of a combined sewer system.

The layout of the outlet section and the location of the installed sensors are represented in Fig. 3. The outlet features:

- A rectangular inlet channel, p_1 (width 3 m, height 3 m), which conveys the mixed sewage from the UDS: the flow rate was measured in this section (s_1) and the stage-discharge curve was derived.
- A side weir (Fig. 3) overflow structure with a crest height of 0.85 m, and length of 4.40 m, which discharges excess flow, activating at around $2 \frac{\text{m}^3}{\text{s}}$. The water level and the quality parameters were measured in this section (s_2).

- A rectangular channel, p_2 (width 3 m, height 3 m), which conveys the untreated water discharged during CSOs, to the sea. The water level was measured in this channel (s_3).
- A transverse gate valve with a rectangular opening (width 1.5 m, height 0.7 m).
- A rectangular channel, p_3 (width 1.5 m, height 3 m), which conveys the sewage to the pumping station (and then, to the WTP).

A multi-parameter probe (Aquaread® AP-5000) was installed in front of the side weir (s_2) (Fig. 4), inside a protective pipe, in a place where sediment accumulation over time did not occur. In this way, it could be safely assumed that the parameter values measured by the probe were the same of the discharged water (owing to complete mixing of the flow). Nonetheless, a regular cleaning protocol of the probe was defined, executed once a week to keep the probe head free from sediments and biological film. A testing period preceded the start of the monitoring campaign, during which the electric and optical sensors of the probe were calibrated following the manufacturer user manual. Frequent checks and re-calibrations were also carried out to ensure the reliability of the quality measurements over time.

Raw data of electrical conductivity (EC), temperature, water level, dissolved oxygen (DO), and turbidity, were measured continuously, transmitted via a modem, and stored remotely. Total dissolved solids (TDS) were estimated from EC and temperature through an empirical relationship (e.g., Atekwana et al., 2004; Taylor et al., 2018; Walton, 1989). To ensure the reliability of the data, they were pre-processed and cleaned from negative values (when applicable), outliers, and unrealistic spikes; parameter values measured by the probe were periodically compared with samples collected in front of the side weir and analysed in laboratory. Based on these measurements, among the estimates of pollutants derived from the data acquired by the electrical sensor and the optical sensor, TDS and DO were found to be the most reliable, as they showed plausible trends during both dry and wet weather. Differently, despite the frequent cleaning of the probe optics, the measurements from the turbidity sensor were often unreliable, likewise the estimates of nitrogen compounds. Therefore, TDS and DO concentrations were chosen as water quality parameters suitable to be modelled.

In the inlet channel (s_1), flow rate was measured with a laser/ultrasonic sensor (TIENet® 360 LaserFlow®), while in front of the side weir (s_2) and in the overflow channel (s_3), water levels were measured with pressure sensors (SIEMENS® Sitrans P). The average measured dry weather flow at s_1 was $0.090 \frac{\text{m}^3}{\text{s}}$. A list of the sensor technical specifications and the measured parameters is provided in Table 2.

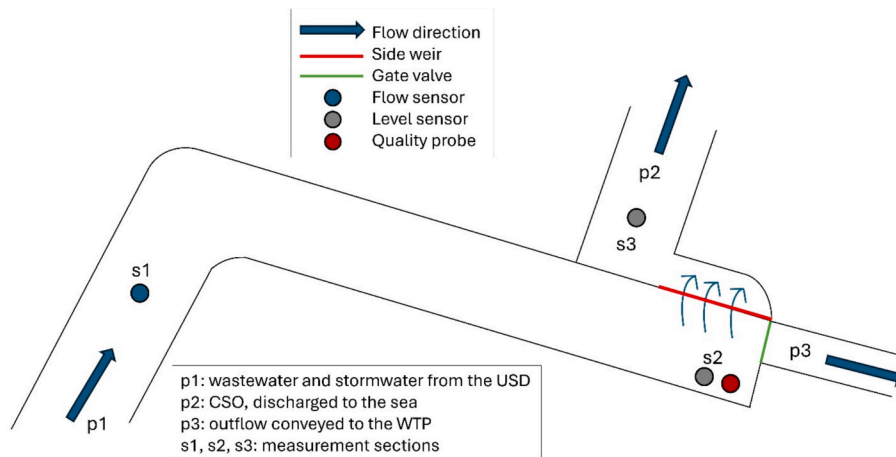


Fig. 3. Layout of the main outlet of the UDS of Portici, where sensors for online measurements were installed. Three measurement sections were instrumented to record water quality (s_2) and quantity (s_1 , s_2 , and s_3) data.



Fig. 4. Overflow structure (s_2), where the water quality multi-parameter probe was installed. The probe was placed inside a pipe to protect it from damage. The side weir, at the centre of the picture; the gate valve, on the right of the picture.

Table 2

List of sensor technical specifications and measured parameters.

Measurement section	Sensor	Exercise temperature	Type of sensor	Measured parameter	Measurement range	Accuracy from actual value
s_1	TIENet® 360 LaserFlow®	$[-20; 60]^{\circ}\text{C}$	Laser	Velocity $\left[\frac{\text{m}}{\text{s}}\right]$	$[-4.6; 4.6]$	± 0.03
s_2	Aquaread® AP-5000	$[-5; 50]^{\circ}\text{C}$	Ultrasonic	Level [m]	$[0; 3]$	± 0.012
			Electric	EC ^a $\left[\frac{\mu\text{S}}{\text{cm}}\right]$	$[0; 200000]$	± 1
				Temperature $^{\circ}\text{C}$	$[-5; 50]$	± 0.1
				Level [m]	$[0; 60]$	$\pm 0.2\%$
				TDS [mg/L]	$[0; 9999]$	$\pm 1\%$
			Optical (1)	DO ^b $\left[\frac{\text{mg}}{\text{L}}\right]$	$[0; 50]$	$\pm 1\%$
s_3	SIEMENS® Sitrans P	$[-10; 80]^{\circ}\text{C}$	Optical (2)	Turbidity [NTU] ^c	$[0; 3000]$	$\pm 5\%$
			Pressure transducer	Level [m]	$[0; 4]$	$\pm 0.3\%$
			Pressure transducer	Level [m]	$[0; 4]$	$\pm 0.3\%$
			Pressure transducer	Level [m]	$[0; 4]$	$\pm 0.3\%$

^a Electrical conductivity (EC).

^b Dissolved oxygen (DO).

^c Nephelometric turbidity units (NTU).

2.7. Setting up of hydrologic and water quality models

As mentioned in Section 2.3, hydrologic parameters of the semi-distributed model should be obtained through calibration. Specifically, hydrographs measured by s_1 sensors were used as targets for model parameter identification. Seven overflow events were considered, selecting those having hydrographs that could be undoubtedly coupled with measured rainfall. The first five events were used for model training, while the last two for validation. Table 3 reports the main characteristics of the selected events, all characterized by ordinary rainfall intensity, with return periods smaller than two years.

The identified parameters, along with their calibration ranges, are given in Table 4. The parameters n and d_s of the pervious surfaces have little influence on hydrograph evaluation in urban areas (Farina et al., 2022, 2023), as runoff mostly originates from the impervious parts of the sub-catchments during short rainfall events. For the same reason, also the calculated concentration of compounds is not significantly affected by the water quality of the runoff from the pervious surfaces. Therefore, the parameters listed in Table 4 were calibrated for the impervious parts and assumed equal to those of the pervious parts for all the sub-catchments.

Table 3

Overflow events considered for hydrologic and water quality model training and validation.

Event nr.	Date	Duration (min)	Rainfall depth (mm)	Nr. of antecedent dry days	Modelling phase
1	8 July 2022	90	20.8	21	Training
2	16 August 2022	60	22.4	3.25	Training
3	28 August 2022	20	8.0	5	Training
4	1 September 2022	470	18.0	3.25	Training
5	9 September 2022	40	12.2	4.5	Training
6	16 September 2022	210	15.2	5.5	Validation
7	17 September 2022	160	13.6	0.5	Validation

Table 4

Ranges of hydrologic parameters of the semi-distributed model.

Parameter	Calibration range
ΔI	$[-25; +25]\%$
$k = \frac{1}{n}$	$[10; 100] \frac{\text{m}^{1/3}}{\text{s}}$
d_s	$[1.25; 5.0] \text{ mm}$

For each sub-catchment, the calibration of the semi-distributed model involves the identification of the three hydrologic parameters listed in Table 4, within the reported intervals, which were defined in such a way to contain all their plausible values. Regarding I , its starting guess values were estimated from the maps for each sub-catchment, and then the deviations ΔI from the starting guess were calibrated. Hence, the values of 99 parameters had to be identified.

Regarding the water quality, for the TDS, which is affected by build-up and wash-off processes, the parameters C_1 , C_2 , C_3 and C_4 of Eqs. (6) and (7) were calibrated, within ranges consistent with literature values (e.g., Hossain et al., 2010; Tu & Smith, 2018; Wicke et al., 2012). Furthermore, $C_W = 900 \frac{\text{mg}}{\text{l}}$ was assumed as the average TDS estimated with the multiparametric probe during dry weather flow, and $C_R = 10 \frac{\text{mg}}{\text{l}}$ was assumed from literature values for rainfall, as representative of the conditions of the wastewater prior to the wash-off process (Beysens et al., 2017; Jawad Al Obaidy & Joshi, 2006; Madhushani et al., 2023). Chemical reactions affecting the concentration of TDS have been neglected, thus $K_1 = 0$ has been assumed in Eq. (4).

For the DO, build-up and wash-off were neglected (i.e., Eqs. (6) and (7) were not applied), but the oxidation of the organic matter transported by the wastewater had to be considered. Hence, in Eq. (4), the reaction constant K_1 was calibrated, while the inflow concentration was calculated as the result of the mixing of runoff and wastewater. To this aim, $C_W = 0 \frac{\text{mg}}{\text{l}}$ was assumed, since during dry weather conditions the measured DO was always $< 0.5 \frac{\text{mg}}{\text{l}}$, and C_R was calibrated in the range $[0; 20] \frac{\text{mg}}{\text{l}}$ (Gee et al., 2021). Table 5 reports the calibrated water quality parameters and the adopted calibration ranges.

Rather than performing a rigorous calibration of the model, a Monte Carlo sampling technique was adopted to run a model sensitivity analysis, generating 10,000 parameter sets by randomly sampling the same number of values from a uniform distribution within the assumed ranges of the parameters. The GoF between observed and simulated hydrograph, TDS graph, and DO graph, was evaluated through the Normalised Nash-Sutcliffe Efficiency ($NNSE$) coefficient (Mathevet et al., 2006). The Nash-Sutcliffe Efficiency coefficient (NSE , Nash & Sutcliffe, 1970) and the $NNSE$ are defined as follows:

$$NSE = 1 - \frac{\sum_{t=1}^T (y_{obs}^t - y_{sim}^t)^2}{\sum_{t=1}^T (y_{obs}^t - \bar{y}_{obs})^2} \quad (8)$$

Table 5

Calibrated water quality parameters of the lumped model.

Parameter	Calibration range
Water quality parameters (TDS)	
$C_1 \left(\frac{\text{kg}}{\text{ha}} \right)$	$[0; 150]$
$C_2 \left(\frac{1}{\text{d}} \right)$	$[1.0; 1.8]$
$C_3 \left(\frac{\text{d}^{C_4-1}}{\text{m}^{C_4}} \right)$	$[0.0; 0.3]$
$C_4 (-)$	$[0.3; 1.0]$
Water quality parameters (DO)	
$C_R \left(\frac{\text{mg}}{\text{l}} \right)$	$[0; 20]$
$K_1 \left(\frac{1}{\text{d}} \right)$	$[0; 2500]$

$$NNSE = \frac{1}{2 - NSE} \quad (9)$$

where y_{obs}^t and y_{sim}^t are respectively the observed and the simulated values of the generic quantity y , at the time step t , \bar{y}_{obs} is the mean of observed value of y , and T is the number of discretization steps of the time series of y . The $NNSE$ of hydrograph ($NNSE_Q$), TDS graph ($NNSE_{TDS}$) and DO graph ($NNSE_{DO}$), were evaluated by running SWMM simulations, with the different sets of the sampled values of model parameters. For the evaluation of the GoF, the values of $NNSE_Q$, $NNSE_{TDS}$, and $NNSE_{DO}$ were evaluated both for single events (i.e., event-specific calibration) and averaged among the five overflow events considered for model training.

3. Results

3.1. Hydrologic results

Among the 10,000 parameter sets of the Monte Carlo sampling for the semi-distributed model, the best GoF was 0.863 for the training set, corresponding to 0.818 and 0.703 for events nr. 6 and nr. 7 (i.e., validation dataset). The model performance was generally good, as indicated by Fig. 5a, where the scatter plot of the $NNSE_Q$ values, averaged among all the seven overflow events, of the 10,000 randomly generated parameter sets is plotted.

The spreading of the values of $NNSE_Q$ is relatively limited, as indicated by the frequency histogram given in Fig. 5b, which shows that about 90 % of the generated parameter sets led to $NNSE_Q$ between 0.760 and 0.813. In the same graphs of Fig. 5, the value of $NNSE_Q = 0.816$, obtained with the uncalibrated lumped hydrologic model, is also indicated.

The performance of the uncalibrated lumped model was indeed also good, with values of $NNSE_Q$ comparable, and in some cases even higher, than those of the semi-distributed model. The observed and simulated hydrographs, for all the considered rainfall events, are represented in Fig. A1 of the Appendix. As an example, Fig. 6 shows the best reproduced event of the training dataset, event nr. 1, and the worst reproduced event of the validation dataset, event nr. 7. The hydrograph of event nr. 1 is very well reproduced with the semi-distributed model ($NNSE_Q = 0.883$), as well as with the uncalibrated lumped model, which in this case performs even better ($NNSE_Q = 0.933$). For event nr. 7, the performance worsens, as it results in $NNSE_Q = 0.703$ with the semi-distributed model and $NNSE_Q = 0.679$ with the uncalibrated lumped model. However, even in this case the results of the simulations can be considered satisfactory, given that the event was different from all the others of the dataset, as it was characterized by a very short dry period before its beginning and by a small rain intensity (Table 3). The good performance of the lumped model was confirmed by the $NNSE_Q = 0.826$ obtained for event nr. 6 of the validation set, which was even slightly better than the value obtained with the semi-distributed model.

3.2. Water quality results

The identification of the parameters related to water quality modelling was carried out by considering the sample that corresponded to the highest values of $NNSE_{DO}$ and $NNSE_{TDS}$. Specifically, the two indexes were calculated either as the mean of the five events of the training set, or by considering each event separately. The obtained parameter values are given in Table 6, while Table 7 reports the corresponding best values of $NNSE_{DO}$ and $NNSE_{TDS}$. Although for most of the considered events the identified parameters have similar values, there are some exceptions, indicating that in some cases the best simulation of the observed concentration with the adopted equations would require event-specific calibration.

However, random sampling of the water quality parameters led to

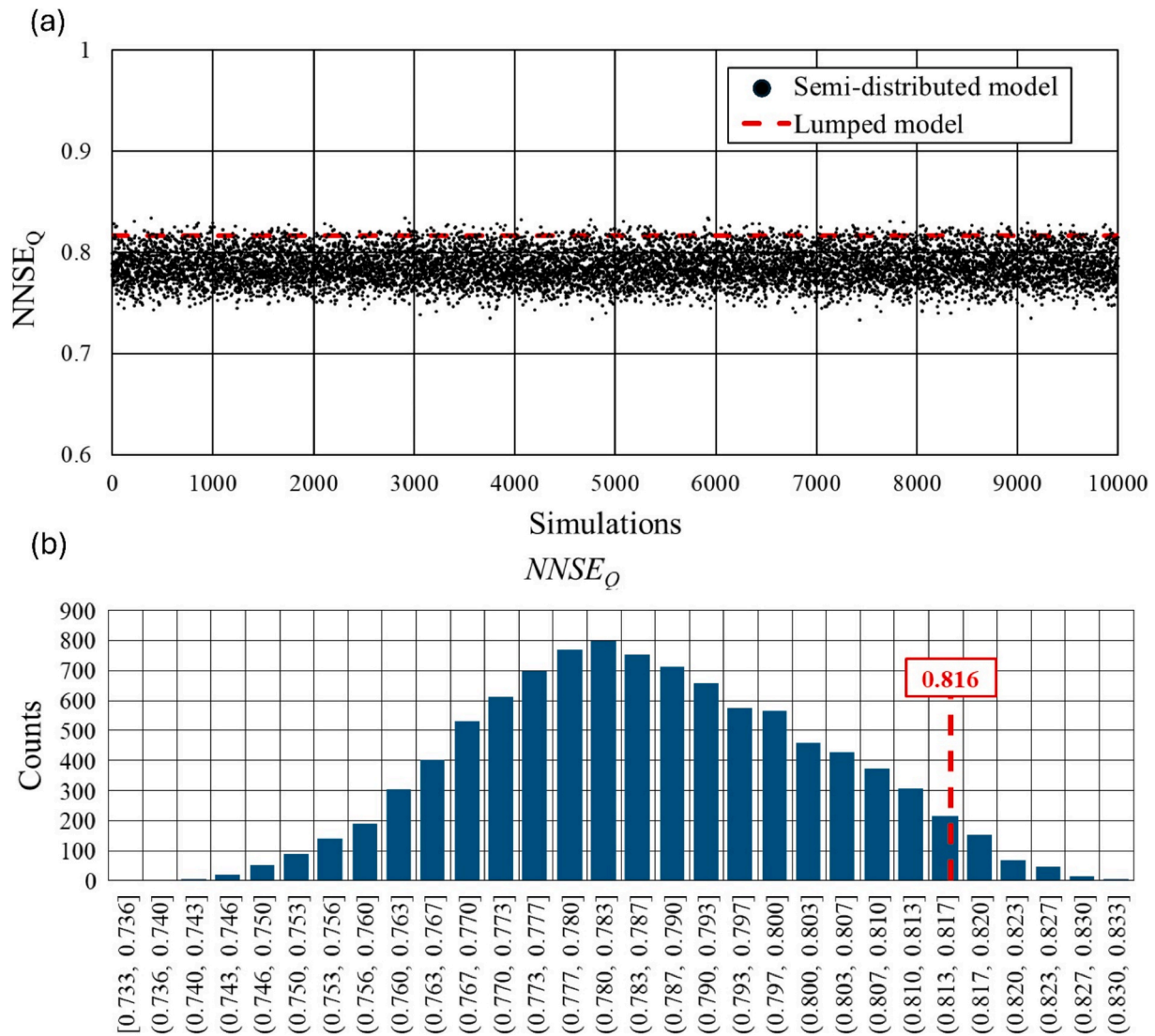


Fig. 5. Goodness of fit of the hydrologic simulations averaged among all the seven runoff events: (a) scatter plot of the $NNSE_Q$ values of the semi-distributed model with 10,000 randomly generated parameter sets; (b) frequency distribution of the $NNSE_Q$ values of the semi-distributed model with 10,000 randomly generated parameter sets ($NNSE_Q$ are evaluated as the average among seven events). The dashed red lines represent the $NNSE_Q$ obtained with the uncalibrated lumped hydrologic model. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

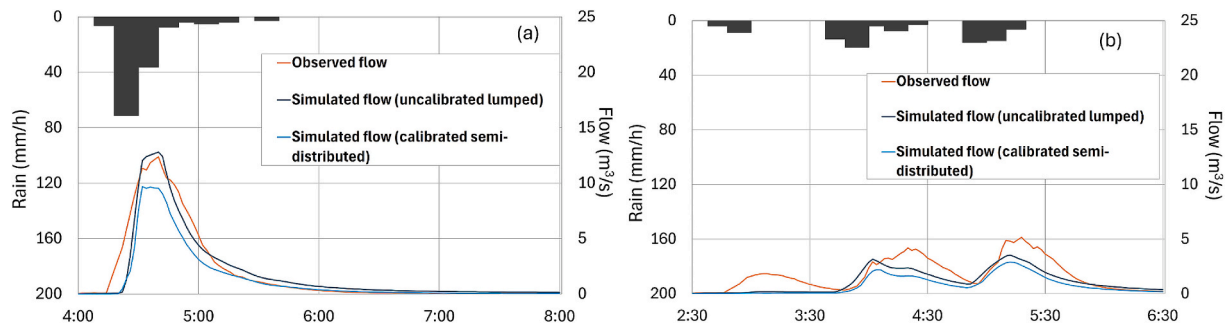


Fig. 6. Example of observed hydrographs vs. hydrographs simulated with both the uncalibrated lumped model and with the best-performing sampled parameter set of the semi-distributed model: (a) event nr. 1 (best reproduced event of the training dataset); (b) event nr. 7 (worst reproduced event of the validation dataset).

reliable simulations of both TDS (for most events) and DO (for some of the events). This result indicates that the lumped approach is suitable to simulate water quality in combined sewer networks. However, while the transport of a conservative species such as TDS, subject to build-up and wash-off processes, is generally well represented, the simulation of the

DO with the complete mixing and the first-order reaction cannot reproduce some of the observed data. As an example, Fig. 7 and Fig. 8 show the simulated concentration graphs compared to the measured ones for the modelled events of the validation dataset (i.e., events nr. 6 and nr. 7). For DO, event nr. 6 achieved $NNSE_{DO} = 0.58$, and for event

Table 6

Best-performing water quality parameters of the lumped model for the five events of the training set (third column), and for each event separately (columns 4–10).

Simulated substance	Parameter	Best-fitting values							
		Training	Event 1	Event 2	Event 3	Event 4	Event 5	Event 6	Event 7
Total dissolved solids (TDS)	$C_1 \left(\frac{\text{kg}}{\text{ha}} \right)$	61.2	59.6	67.1	30.0	65.2	53.6	63.3	136.0
	$C_2 \left(\frac{1}{\text{d}} \right)$	1.45	1.67	1.48	1.71	1.19	1.07	1.00	1.57
	$C_3 \left(\frac{\text{d}^{C_4-1}}{\text{m}^{C_4}} \right)$	0.114	0.159	0.122	0.271	0.106	0.228	0.091	0.039
Dissolved oxygen (DO)	$C_4 (-)$	0.608	0.649	0.616	0.622	0.540	0.700	0.551	0.731
	$C_R \left(\frac{\text{mg}}{\text{l}} \right)$	8.61	11.7	4.80	0.775	17.4	5.83	10.7	5.27
	$K_1 \left(\frac{1}{\text{d}} \right)$	689.2	870.9	121.9	2453	2492	189.5	2492	138.7

Table 7

Goodness of fit of the best-performing water quality simulations achieved through Monte Carlo sampling of model parameters for the five events of the training set (column 3), for the validation set (column 4), and for each event separately (columns 5–11).

Simulated substance	Metric	Best goodness of fit								
		Training set	Validation set	Event 1	Event 2	Event 3	Event 4	Event 5	Event 6	Event 7
Total dissolved solids (TDS)	$NNSE_{TDS}$	0.75	0.63	0.67	0.77	0.94	0.84	0.85	0.86	0.52
Dissolved oxygen (DO)	$NNSE_{DO}$	0.52	0.58	0.83	0.61	0.54	0.75	0.65	0.66	0.65

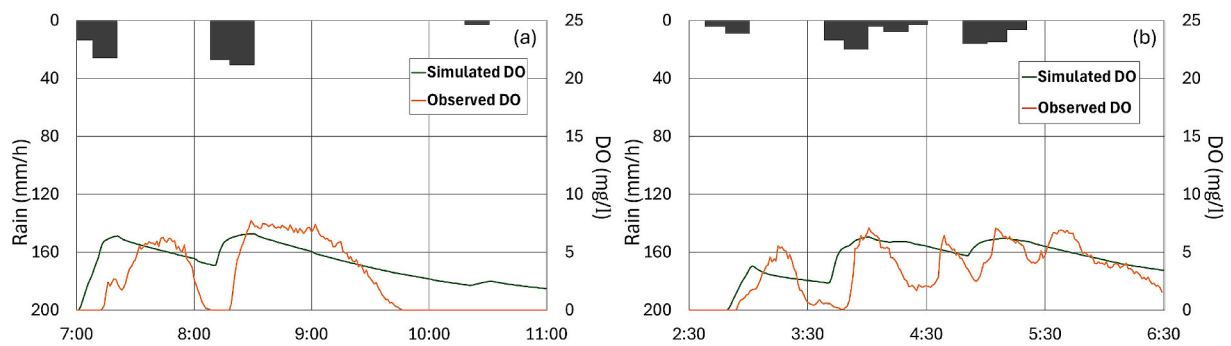


Fig. 7. Examples of simulated vs. observed DO concentration graphs (lumped model of the combined sewer network) for the validation dataset: (a) event nr. 6; (b) event nr. 7.

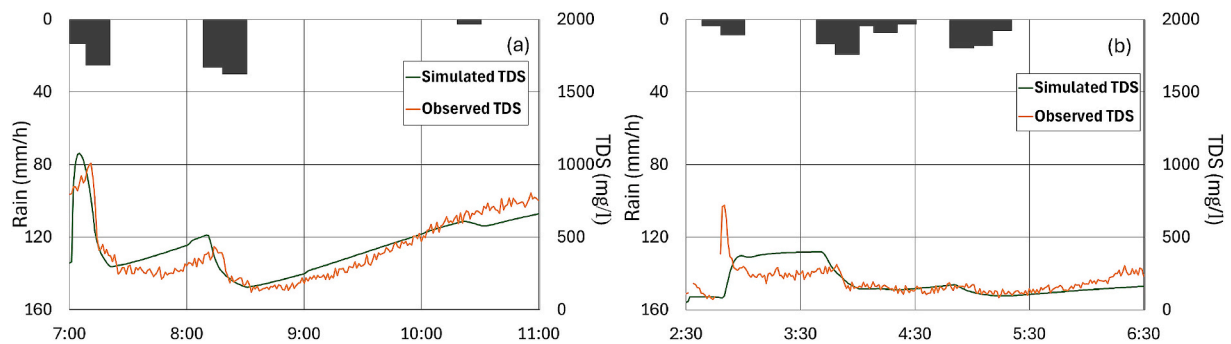


Fig. 8. Examples of simulated vs. observed TDS concentration graphs (lumped model of the combined sewer network) of the validation dataset: (a) event nr. 6; (b) event nr. 7.

nr. 7 it resulted in $NNSE_{DO} = 0.59$. For TDS, event nr. 6 achieved $NNSE_{TDS} = 0.84$, and for event nr. 7 it resulted in $NNSE_{TDS} = 0.41$. The observed and calibrated graphs of DO and TDS concentrations, for the event-specific model calibration, are represented in Fig. A2 and Fig. A3 of the Appendix, respectively.

4. Discussion

The Monte Carlo sampling of the hydrologic parameters of the semi-distributed modelling approach leads to $NNSE_Q$, averaged among the five runoff events considered in the training dataset, as high as 0.863. However, the calibration of the semi-distributed model clearly suffers from equifinality issues, as different parameter sets lead to similar $NNSE_Q$. In this respect, the values of the correlation indexes between the parameter sets corresponding to the ten best simulations (i.e., those with the highest values of $NNSE_Q$) are reported in Table 8. In all cases, the correlation among the parameter sets is quite low. This result indicates that the best-performing ten sets of sampled parameters, though leading to very similar values of $NNSE_Q$ averaged among all the seven events (i.e., all between 0.830 and 0.834), are completely different one from each other. This result points out the ill-posedness of the parameter identification problem for the semi-distributed hydrologic model. The variations of hydrologic parameters of single sub-catchments balance each other out, only slightly affecting the simulated hydrograph at the outlet.

Regarding the uncalibrated lumped approach, the results clearly indicate its suitability for reliable simulations of stormwater hydrographs. The model, with the hydrologic parameters of Table 1 estimated from cartographic information with the relationships proposed by Farina et al. (2023), provides surprisingly good results (see Fig. 6 and Fig. A1 of the Appendix), with $NNSE_Q$ ranging between 0.68 and 0.93 for the seven events. The value of $NNSE_Q = 0.842$, averaged among the five events of the training set, is close to $NNSE_Q = 0.863$, i.e. the highest achieved with the semi-distributed model with the Monte Carlo sampling method. Although this latter allows slightly improving the performance of the simulations, the computational burden of calibration, and the issue of equifinality of the parameters, hamper its general applicability. Hence, the lumped hydrologic approach represents quite a useful tool for the management of combined sewer systems, especially in absence of measurements of water flow to be used for model calibration.

Differently, the application of the simplified simulation of water quality within the lumped approach, though giving satisfactory results for many of the considered events (see the $NNSE_{TDS}$ and $NNSE_{DO}$ values given in Table 7), presents some issues. It is worth to note, however, that the sensors of the multiparametric probe only indirectly measure DO and TDS. Respectively, DO is obtained from optical measurements, and TDS concentration from electrical conductivity measurements. In both cases, empirical relationships developed by the manufacturer are employed to convert the measured quantity into the desired parameter. This empirical conversion surely increases the uncertainty of the estimated concentrations, and thus their reproducibility with model simulations.

As indicated by the identified parameters given in Table 6, for both

DO and TDS, the best-fitting parameter sets exhibit significant differences among the considered events. While these differences are relatively small for the four parameters of the build-up and wash-off equations for TDS simulation, this issue is particularly relevant for DO simulations, where very different values of the same water quality parameters are identified for some of the events. For instance, Table 6 reports $C_R = 0.775$ mg/l for event 3 and $C_R = 17.4$ mg/l for event 4. Similarly, it results in $K_1 = 121.9$ d⁻¹ for event 2 and $K_1 = 2492$ d⁻¹ for event 4. Indeed, the comparison of simulated and observed DO concentrations (Fig. 7 and Fig. A2 of the Appendix) shows that, in most cases, a delay of the DO concentration increase, compared to discharge growth, is observed. This delay seems related to the position of the peak in the precipitation input histogram, and it affects the calculated $NNSE_{DO}$ in such a way that the best-fitting simulated DO concentration does not reproduce the observed fluctuations, but it rather follows a smooth trend in between them (e.g., Fig. 7b). The smoothening of the fluctuations leads in some cases to the identification of unfeasible high values of the reaction constant K_1 .

This issue clearly affects the identifiability of parameter values holding for all the events. Fig. 9 and Fig. 10 show the dependence of $NNSE_{TDS}$ and $NNSE_{DO}$, averaged over the seven modelled events, on the calibrated parameters of water quality model for the two species. Regarding $NNSE_{TDS}$, it shows some sensitivity to the coefficient C_1 of build-up equation up to the value of about 61 kg/ha, while it is nearly unaffected by the exponent C_2 throughout the entire investigated interval. Regarding the parameters of the wash-off equation, the simulations are sensitive to the exponent coefficient C_4 , with a maximum around $C_4 = 0.61$. Instead, the dependence on parameter C_3 is very flat around the maximum.

Similarly, the results of the simulations of DO indicate very little sensitivity to both the parameters, although $NNSE_{DO}$ shows a maximum around $C_R = 8.6$ mg/l (Fig. 10a). The first-order reaction coefficient K_1 , instead, only slightly affects the fitting of the simulations for values larger than 1500 d⁻¹ (Fig. 10b). As already pointed out, this result is related to the incapability of the model to catch the timing of the DO concentration rise after the rainfall events, in turn affecting the unfeasible identified high values of K_1 .

The limited sensitivity to parameter variations of the simulated concentrations points out that the water quality model, based on Eqs. (4)–(7), does not consider all the factors affecting the mixing and transport processes of the simulated species in the sewer network, as also indicated by the contrasting values of the same parameter obtained in some cases after the calibration.

Although more data would be needed to give a possible explanation for these results, it is worth noticing that the characteristics of rainfall events clearly affect the initial DO concentration in the runoff, where oxidation reactions likely occur, which may affect the dissolved oxygen concentration and are not considered in the model. In this respect, Fig. 11 shows the dependence of the identified DO runoff concentration C_R on the total rainfall depth of the considered events, showing a peak around 18 mm.

Fig. 12 shows how the identified values of the parameters C_1 (build-

Table 8

Correlation matrix of the ten parameter sets leading to the highest values of average $NNSE_Q$ with the semi-distributed hydrologic approach.

Parameter set	Set 1	Set 2	Set 3	Set 4	Set 5	Set 6	Set 7	Set 8	Set 9	Set 10
Set 1	1.00	0.38	-0.04	0.39	0.38	0.39	0.25	-0.16	0.12	0.29
Set 2	0.38	1.00	-0.21	0.35	0.26	0.32	0.13	0.37	0.29	0.05
Set 3	-0.04	-0.21	1.00	-0.06	0.00	0.21	0.24	0.23	0.16	0.35
Set 4	0.39	0.35	-0.06	1.00	0.47	0.25	0.11	0.27	0.24	0.08
Set 5	0.38	0.26	0.00	0.47	1.00	0.67	-0.01	0.05	0.09	0.03
Set 6	0.39	0.32	0.21	0.25	0.67	1.00	0.19	0.15	0.13	0.24
Set 7	0.25	0.13	0.24	0.11	-0.01	0.19	1.00	-0.05	0.35	0.27
Set 8	-0.16	0.37	0.23	0.27	0.05	0.15	-0.05	1.00	0.25	0.01
Set 9	0.12	0.29	0.16	0.24	0.09	0.13	0.35	0.25	1.00	0.02
Set 10	0.29	0.05	0.35	0.08	0.03	0.24	0.27	0.01	0.02	1.00

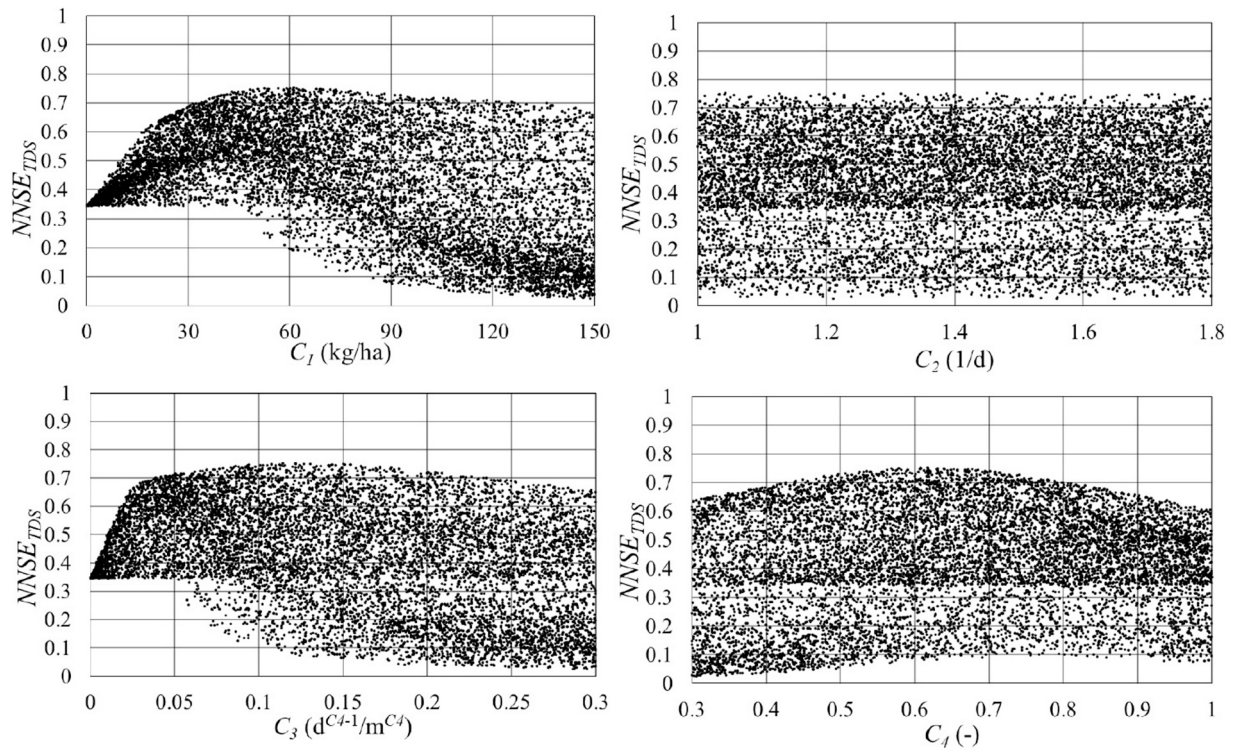


Fig. 9. Dependence of the $NNSE_{TDS}$ values, averaged over the five events of the training set, on the water quality parameters, based on the simulations carried out with the lumped model for the 10,000 randomly generated sets of water quality parameter values.

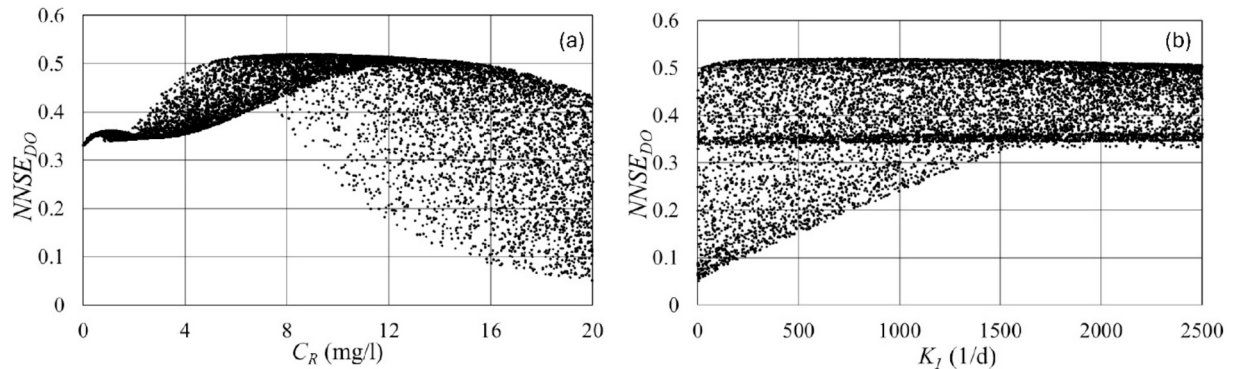


Fig. 10. Dependence of the $NNSE_{DO}$ values, averaged over the five events of the training set, on the water quality parameters, based on the simulations carried out with the lumped model for the 10,000 randomly generated sets of water quality parameter values.

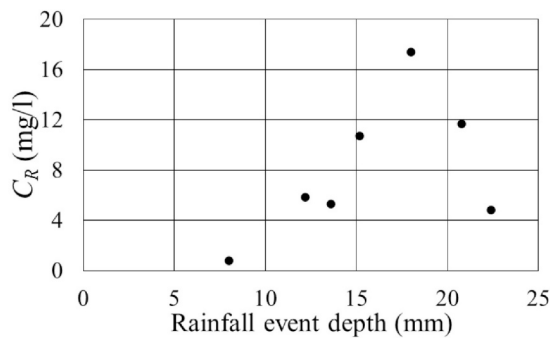


Fig. 11. Scatter plot of DO concentration in the runoff C_R vs. the total rainfall depth of each event.

up equation) and C_3 (wash-off equation) are affected by the duration of the dry period before the onset of each rain event, respectively suggesting decreasing and increasing trends for antecedent dry intervals up to 5 days. However, more events and further elaborations would be required to shed more light in these modelling issues.

5. Conclusions

Reliable mathematical models of water quantity and quality in combined sewer networks are essential for their management. In this paper, the performance of hydrologic semi-distributed and lumped models, both developed in SWMM, have been compared for the case study of the city of Portici (Italy). Then, the lumped model has been applied to the simulation of water quality. High-resolution online measurements of discharge, carried out with a laser/ultrasonic sensor, and of several water quality parameters, acquired through a multi-parametric probe, were available at the outlet of the network.

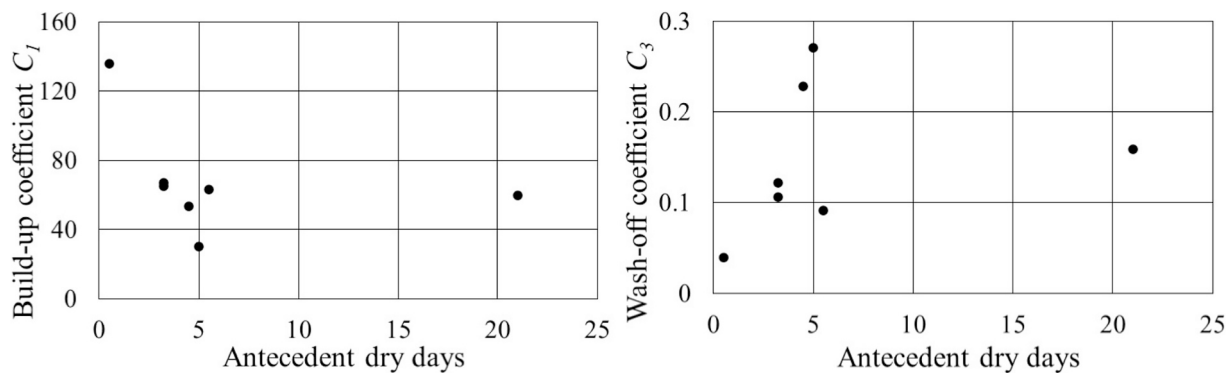


Fig. 12. Scatter plot of the identified parameters C_1 and C_3 of TDS build-up and wash-off equations vs. the duration of the dry interval preceding each rain event.

Discharge data allowed the sensitivity of the semi-distributed hydrological model to the variations of its 99 unknown parameters. The results indicate that the semi-distributed model can provide reliable simulation of the measured hydrographs, but the inverse problem of parameter identification was affected by equifinality, thus impeding the identification of parameters with general validity, i.e. applicable also in absence of measurements. Differently, the lumped model of the network was set up without calibration, thanks to the empirical relationships recently proposed by Farina et al. (2023) for the estimation of its hydrologic parameters directly from cartographic information. The hydrographs simulated either with the uncalibrated lumped model or with the best-performing sampled parameter sets with the semi-distributed model are both close to the experimental ones. This result confirms the suitability of the lumped modelling approach of Farina et al. (2023) for the development of reliable hydrologic models of combined sewer networks, especially when discharge measurements are not available.

The lumped approach was then applied to the modelling of water quality in the network, specifically simulating the measured concentrations of dissolved oxygen (DO) and total dissolved solids (TDS). Owing to the oxidization of organic matter when wastewater mixed with runoff, DO was modelled as a reactive transported species with a simplified first-order reaction rate, with the reaction constant treated as a model calibration parameter. Differently, TDS were considered conservative. For the modelling of TDS transport, build-up and wash-off phenomena were also considered. Empirical exponential equations were adopted for their modelling, the parameters of which had to be calibrated for the case study.

The calibration of the water quality parameters led to reliable simulations of the measured concentrations during most of the observed runoff events, especially for TDS. This result indicates that lumped approach with simplified in-sewer process simulation is suitable for UDS modelling, and it may be used in place of commonly adopted more complex approaches (Rodríguez et al., 2013). However, further investigations are required to understand issues affecting the simulations of DO in some of the events. Furthermore, different sets of water quality parameters were identified for some events. This issue highlights the complexity of water quality dynamics in combined sewers, affected by event-specific factors which cannot be completely captured by

simplified approaches such as first-order reactions or exponential build-up and wash-off equations. This result highlights the need for data from continuous monitoring of wastewater quality in sewers, such as this presented in this study, which will help develop reliable modelling approaches.

CRediT authorship contribution statement

Pasquale Marino: Writing – review & editing, Writing – original draft, Validation, Software, Methodology. **Alessandro Farina:** Software, Data curation. **Rudy Gargano:** Writing – review & editing, Supervision, Methodology, Conceptualization. **Zoran Kapelan:** Writing – review & editing, Supervision, Methodology, Conceptualization. **Jeroen Langeveld:** Writing – review & editing, Supervision, Conceptualization. **Roberto Greco:** Writing – review & editing, Supervision, Methodology, Funding acquisition, Conceptualization.

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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 1

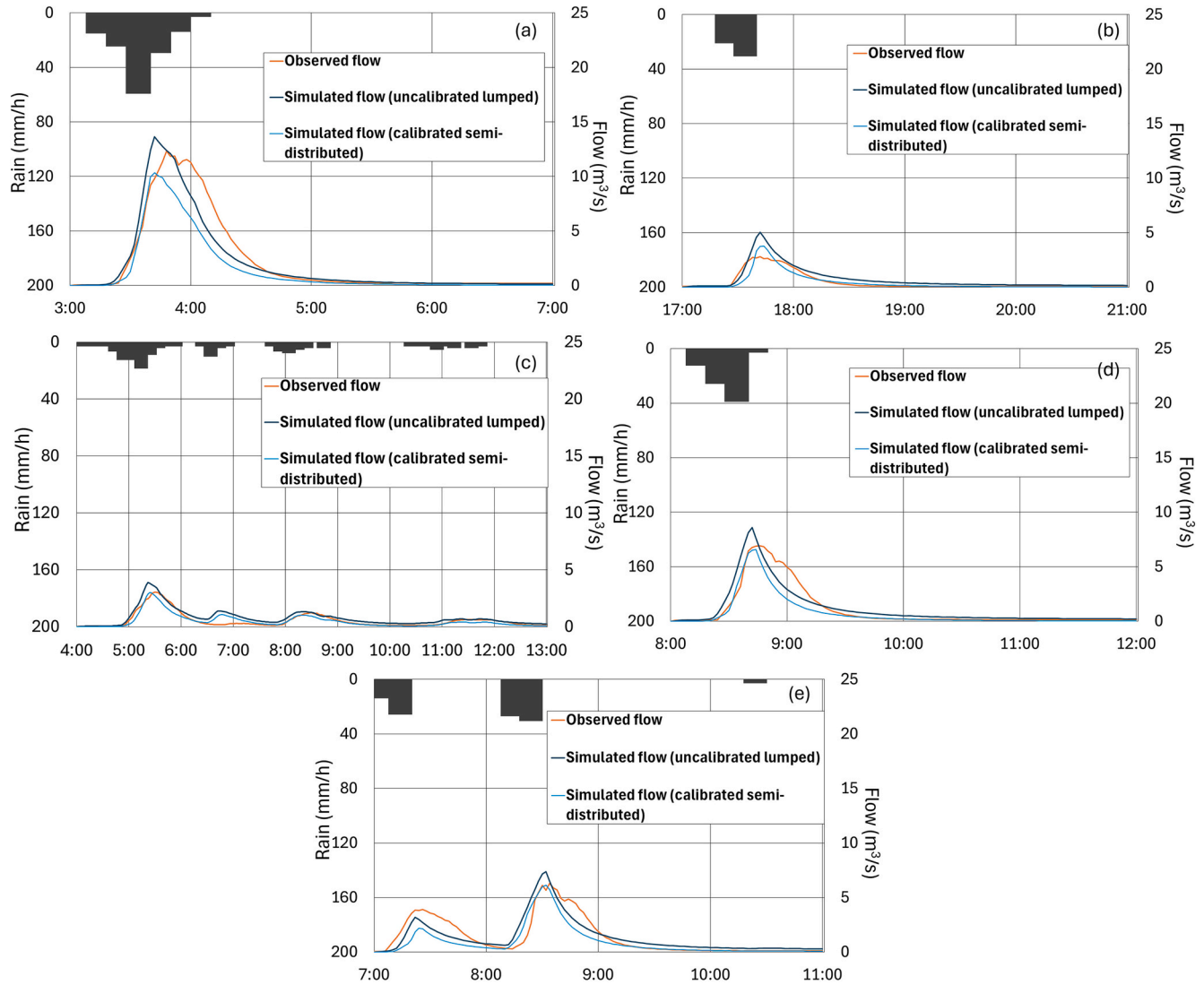


Fig. A1. Observed hydrographs vs. hydrographs simulated with both the uncalibrated lumped model and with the calibrated semi-distributed model: (a) event nr. 2; (b) event nr. 3; (c) event nr. 4; (d) event nr. 5; (e) event nr. 6. Events nr. 2, 3, 4 and 5 belong to the training dataset. Event nr. 6 belongs to the validation dataset.

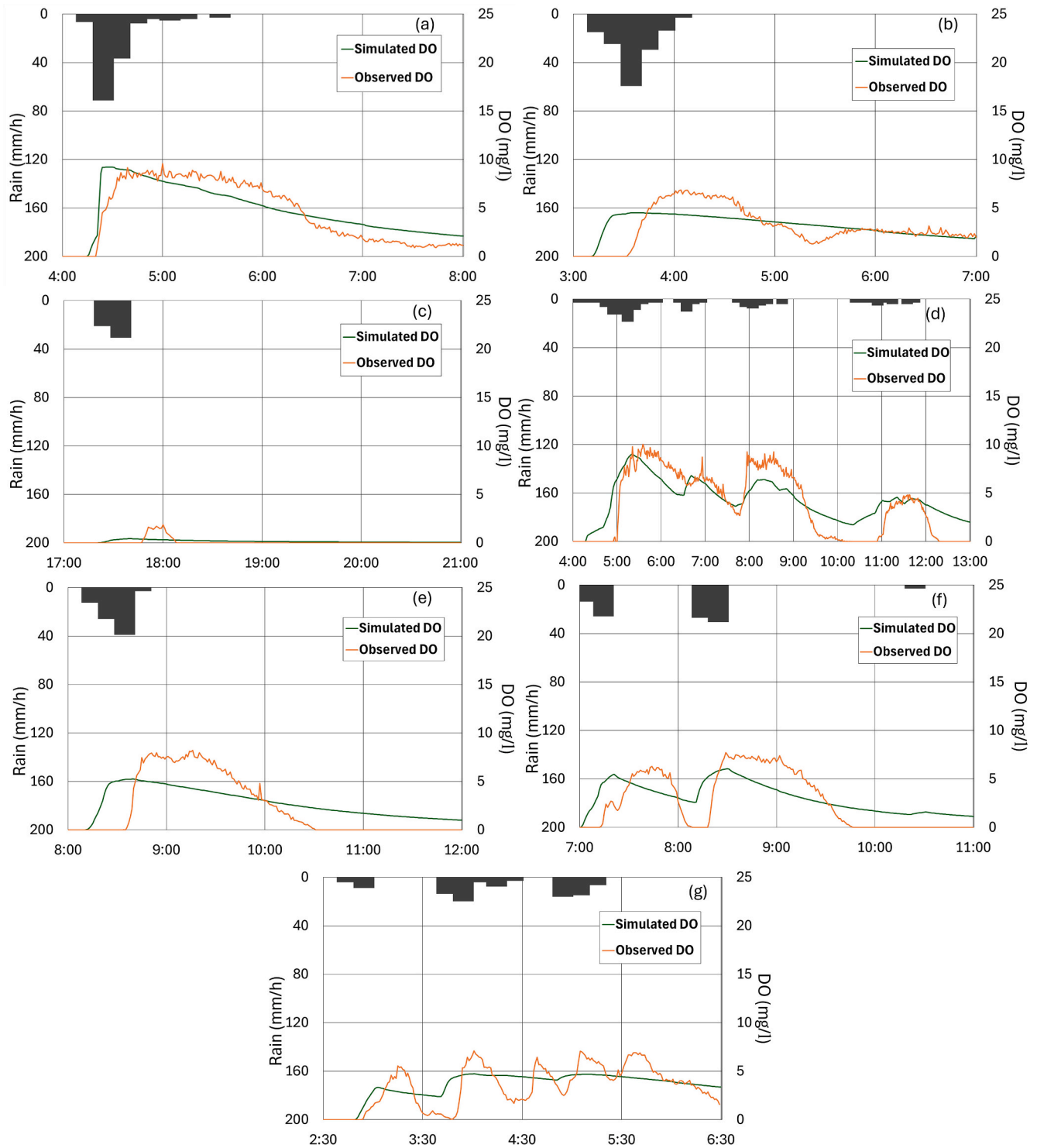


Fig. A2. Observed vs. simulated dissolved oxygen concentrations with event-specific model calibration (simulations carried out with the lumped model of the combined sewer network): (a) event nr. 1; (b) event nr. 2; (c) event nr. 3; (d) event nr. 4; (e) event nr. 5; (f) event nr. 6; (g) event nr. 7.

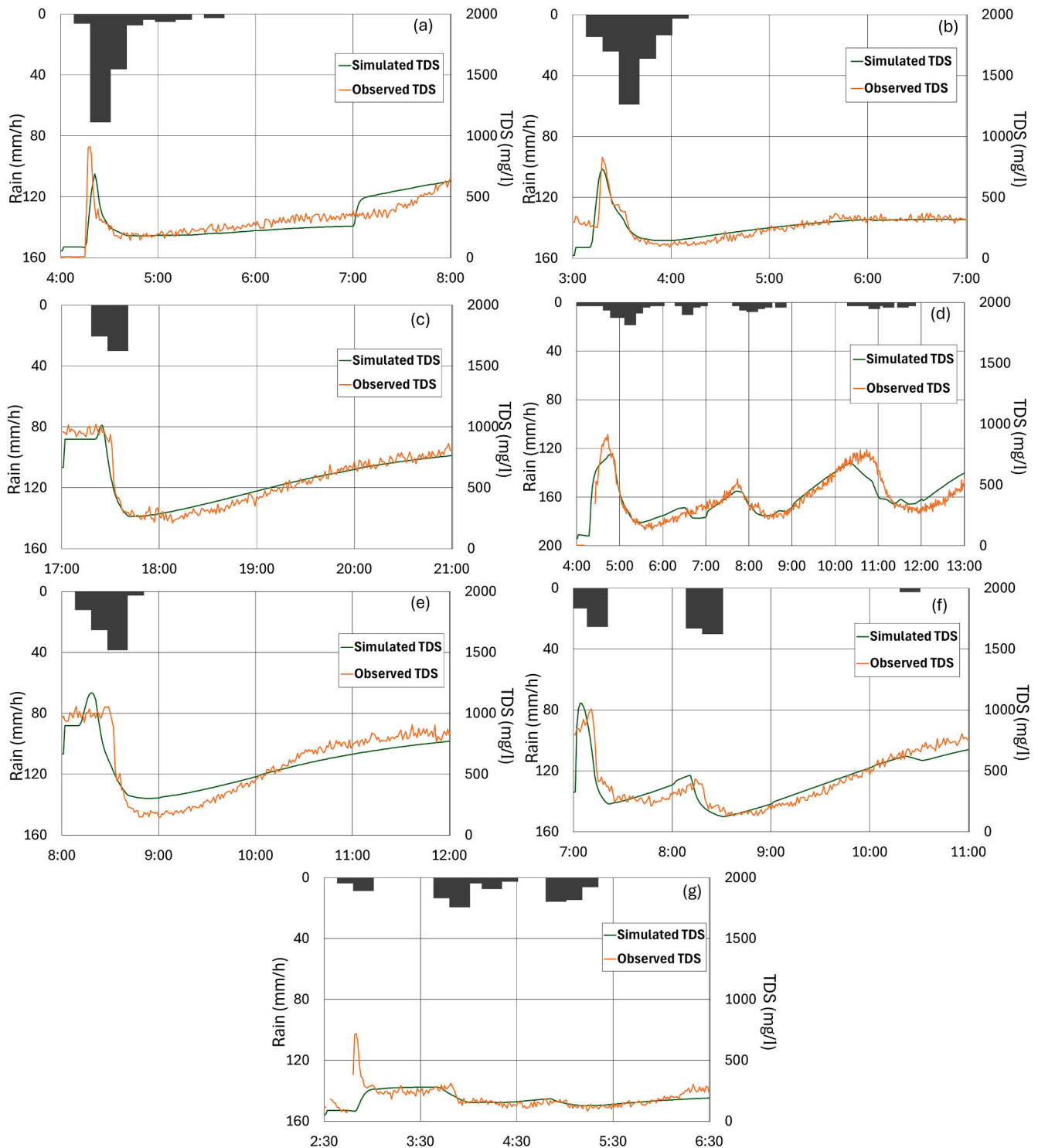


Fig. A3. Observed vs. simulated total dissolved solids concentrations with event-specific model calibration (simulations carried out with the lumped model of the combined sewer network): (a) event nr. 1; (b) event nr. 2; (c) event nr. 3; (d) event nr. 4; (e) event nr. 5; (f) event nr. 6; (g) event nr. 7.

Data availability

All data and files used in the study are available from the corresponding author upon reasonable request.

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